Finite difference methods for wave motion

Hans Petter Langtangen[1,2]

[1]Center for Biomedical Computing, Simula Research Laboratory
[2]Department of Informatics, University of Oslo

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This is still a **preliminary version**.

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A very wide range of physical processes lead to wave motion, where signals re propagated through a medium in space and time, normally with little or o permanent movement of the medium itself. The shape of the signals may ndergo changes as they travel through matter, but usually not so much that ıe signals cannot be recognized at some later point in space and time. Many ypes of wave motion can be described by the equation $u_{tt} = \nabla \cdot (c^2 \nabla u) + f$, hich we will solve in the forthcoming text by finite difference methods.

Simulation of waves on a string

Ve begin our study of wave equations by simulating one-dimensional waves on string, say on a guitar or violin string. Let the string in the deformed state ɔincide with the interval $[0, L]$ on the x axis, and let $u(x, t)$ be the displacement

at time t in the y direction of a point initially at x. The displacement f u is governed by the mathematical model

$$\begin{aligned}
\frac{\partial^2 u}{\partial t^2} &= c^2 \frac{\partial^2 u}{\partial x^2}, && x \in (0, L),\ t \in (0, T] \\
u(x, 0) &= I(x), && x \in [0, L] \\
\frac{\partial}{\partial t} u(x, 0) &= 0, && x \in [0, L] \\
u(0, t) &= 0, && t \in (0, T] \\
u(L, t) &= 0, && t \in (0, T]
\end{aligned}$$

The constant c and the function $I(x)$ must be prescribed.

Equation (1) is known as the one-dimensional *wave equation*. Since tl contains a second-order derivative in time, we need *two initial conditio* (2) specifying the initial shape of the string, $I(x)$, and (3) reflecting t initial velocity of the string is zero. In addition, PDEs need *boundary co* here (4) and (5), specifying that the string is fixed at the ends, i.e., t displacement u is zero.

The solution $u(x, t)$ varies in space and time and describes waves t moving with velocity c to the left and right.

Sometimes we will use a more compact notation for the partial deriva save space:

$$u_t = \frac{\partial u}{\partial t}, \quad u_{tt} = \frac{\partial^2 u}{\partial t^2},$$

and similar expressions for derivatives with respect to other variables. T wave equation can be written compactly as $u_{tt} = c^2 u_{xx}$.

The PDE problem (1)-(5) will now be discretized in space and tir finite difference method.

1.1 Discretizing the domain

The temporal domain $[0, T]$ is represented by a finite number of mesh p

$$0 = t_0 < t_1 < t_2 < \cdots < t_{N_t - 1} < t_{N_t} = T\,.$$

Similarly, the spatial domain $[0, L]$ is replaced by a set of mesh points

$$0 = x_0 < x_1 < x_2 < \cdots < x_{N_x - 1} < x_{N_x} = L\,.$$

One may view the mesh as two-dimensional in the x, t plane, consisting c (x_i, t_n), with $i = 0, \ldots, N_x$ and $n = 0, \ldots, N_t$.

Uniform meshes. For uniformly distributed mesh points we can introduce ıe constant mesh spacings Δt and Δx. We have that

$$x_i = i\Delta x,\ i = 0, \ldots, N_x, \quad t_i = n\Delta t,\ n = 0, \ldots, N_t\,. \tag{9}$$

Ve also have that $\Delta x = x_i - x_{i-1}$, $i = 1, \ldots, N_x$, and $\Delta t = t_n - t_{n-1}$, $n = \ldots, N_t$. Figure 1 displays a mesh in the x, t plane with $N_t = 5$, $N_x = 5$, and onstant mesh spacings.

.2 The discrete solution

he solution $u(x,t)$ is sought at the mesh points. We introduce the mesh unction u_i^n, which approximates the exact solution at the mesh point (x_i, t_n) or $i = 0, \ldots, N_x$ and $n = 0, \ldots, N_t$. Using the finite difference method, we shall evelop algebraic equations for computing the mesh function. The circles in igure 1 illustrate neighboring mesh points where values of u_i^n are connected hrough an algebraic equation. In this particular case, u_2^1, u_1^2, u_2^2, u_3^2, and u_2^3 are onnected in an algebraic equation associated with the center point $(2, 2)$. The erm *stencil* is often used about the algebraic equation at a mesh point, and the eometry of a typical stencil is illustrated in Figure 1. One also often refers to ıe algebraic equations as *discrete equations*, *(finite) difference equations* or a *nite difference scheme*.

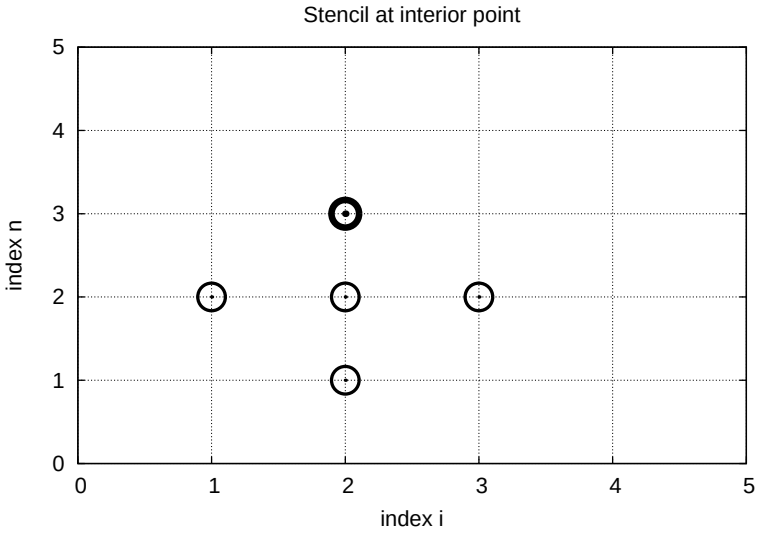


Figure 1: Mesh in space and time for a 1D wave equation.

1.3 Fulfilling the equation at the mesh points

For a numerical solution by the finite difference method, we relax the cc that (1) holds at all points in the space-time domain $(0, L) \times (0, T]$ requirement that the PDE is fulfilled at the *interior* mesh points:

$$\frac{\partial^2}{\partial t^2}u(x_i, t_n) = c^2\frac{\partial^2}{\partial x^2}u(x_i, t_n),$$

for $i = 1, \ldots, N_x - 1$ and $n = 1, \ldots, N_t - 1$. For $n = 0$ we have th conditions $u = I(x)$ and $u_t = 0$, and at the boundaries $i = 0, N_x$ we h boundary condition $u = 0$.

1.4 Replacing derivatives by finite differences

The second-order derivatives can be replaced by central differences. T widely used difference approximation of the second-order derivative is

$$\frac{\partial^2}{\partial t^2}u(x_i, t_n) \approx \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2}\,.$$

It is convenient to introduce the finite difference operator notation

$$[D_t D_t u]_i^n = \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2}\,.$$

A similar approximation of the second-order derivative in the x directic

$$\frac{\partial^2}{\partial x^2}u(x_i, t_n) \approx \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} = [D_x D_x u]_i^n\,.$$

Algebraic version of the PDE. We can now replace the derivative and get

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} = c^2\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2},$$

or written more compactly using the operator notation:

$$[D_t D_t u = c^2 D_x D_x]_i^n\,.$$

Algebraic version of the initial conditions. We also need to rep derivative in the initial condition (3) by a finite difference approxima centered difference of the type

$$\frac{\partial}{\partial t}u(x_i, t_n) \approx \frac{u_i^1 - u_i^{-1}}{2\Delta t} = [D_{2t}u]_i^0,$$

seems appropriate. In operator notation the initial condition is written

$$[D_{2t}u]_i^n = 0, \quad n = 0\,.$$

/riting out this equation and ordering the terms give

$$u_i^{n-1} = u_i^{n+1}, \quad i = 0, \ldots, N_x, \ n = 0\,. \tag{13}$$

he other initial condition can be computed by

$$u_i^0 = I(x_i), \quad i = 0, \ldots, N_x\,.$$

.5 Formulating a recursive algorithm

/e assume that u_i^n and u_i^{n-1} are already computed for $i = 0, \ldots, N_x$. The only nknown quantity in (11) is therefore u_i^{n+1}, which we can solve for:

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + C^2\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right), \tag{14}$$

here we have introduced the parameter

$$C = c\frac{\Delta t}{\Delta x}, \tag{15}$$

nown as the *Courant number*.

C is the key parameter in the discrete diffusion equation.

We see that the discrete version of the PDE features only one parameter, C, which is therefore the key parameter that governs the quality of the numerical solution (see Section 10 for details). Both the primary physical parameter c and the numerical parameters Δx and Δt are lumped together in C. Note that C is a dimensionless parameter.

Given that u_i^{n-1} and u_i^n are computed for $i = 0, \ldots, N_x$, we find new values t the next time level by applying the formula (14) for $i = 1, \ldots, N_x - 1$. Figure 1 lustrates the points that are used to compute u_2^3. For the boundary points, $= 0$ and $i = N_x$, we apply the boundary conditions $u_i^{n+1} = 0$.

A problem with (14) arises when $n = 0$ since the formula for u_i^1 involves u_i^{-1}, hich is an undefined quantity outside the time mesh (and the time domain). owever, we can use the initial condition (13) in combination with (14) when $= 0$ to arrive at a special formula for u_i^1:

$$u_i^1 = u_i^0 - \frac{1}{2}C^2\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)\,. \tag{16}$$

igure 2 illustrates how (16) connects four instead of five points: u_2^1, u_1^0, u_2^0, and $_3^0$.

We can now summarize the computational algorithm:

1. Compute $u_i^0 = I(x_i)$ for $i = 0, \ldots, N_x$

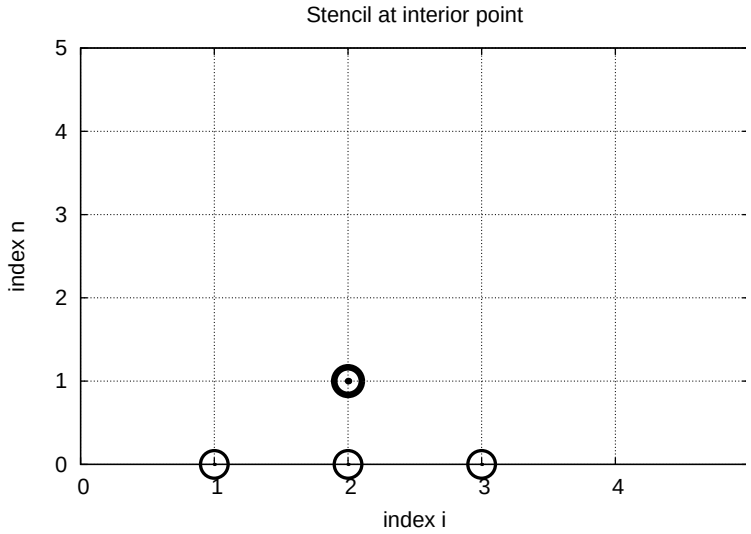


Figure 2: Modified stencil for the first time step.

2. Compute u_i^1 by (16) and set $u_i^1 = 0$ for the boundary points $i =$ $i = N_x$, for $n = 1, 2, \ldots, N - 1$,
3. For each time level $n = 1, 2, \ldots, N_t - 1$
   (a) apply (14) to find u_i^{n+1} for $i = 1, \ldots, N_x - 1$
   (b) set $u_i^{n+1} = 0$ for the boundary points $i = 0$, $i = N_x$.

The algorithm essentially consists of moving a finite difference stencil all the mesh points, which is illustrated by an animation in a web pa movie file[2].

1.6 Sketch of an implementation

In a Python implementation of this algorithm, we use the array elemer to store u_i^{n+1}, `u_1[i]` to store u_i^n, and `u_2[i]` to store u_i^{n-1}. Our convention is use `u` for the unknown new spatial field to be computed the solution at one time step back in time, `u_2` as the solution two tin back in time and so forth.

The algorithm only needs to access the three most recent time level need only three arrays for u_i^{n+1}, u_i^n, and u_i^{n-1}, $i = 0, \ldots, N_x$. Storing solutions in a two-dimensional array of size $(N_x + 1) \times (N_t + 1)$ would be

[1] `http://tinyurl.com/opdfafk/pub/mov-wave/wave1D_PDE_Dirichlet_stencil_g`
[2] `http://tinyurl.com/opdfafk/pub/mov-wave/wave1D_PDE_Dirichlet_stencil_g`

ı this simple one-dimensional PDE problem, but is normally out of the question ı three-dimensional (3D) and large two-dimensional (2D) problems. We shall ıerefore in all our programs for solving PDEs have the unknown in memory at ş few time levels as possible.

The following Python snippet realizes the steps in the computational algo- thm.

```
# Given mesh points as arrays x and t (x[i], t[n])
dx = x[1] - x[0]
dt = t[1] - t[0]
C = c*dt/dx             # Courant number
Nt = len(t)-1
C2 = C**2               # Help variable in the scheme

# Set initial condition u(x,0) = I(x)
for i in range(0, Nx+1):
    u_1[i] = I(x[i])

# Apply special formula for first step, incorporating du/dt=0
for i in range(1, Nx):
    u[i] = u_1[i] - 0.5*C**2(u_1[i+1] - 2*u_1[i] + u_1[i-1])
u[0] = 0;  u[Nx] = 0   # Enforce boundary conditions

# Switch variables before next step
u_2[:], u_1[:] = u_1, u

for n in range(1, Nt):
    # Update all inner mesh points at time t[n+1]
    for i in range(1, Nx):
        u[i] = 2u_1[i] - u_2[i] - \
               C**2(u_1[i+1] - 2*u_1[i] + u_1[i-1])

    # Insert boundary conditions
    u[0] = 0;  u[Nx] = 0

    # Switch variables before next step
    u_2[:], u_1[:] = u_1, u
```

Verification

efore implementing the algorithm, it is convenient to add a source term to the DE (1) since it gives us more freedom in finding test problems for verification. ı particular, the source term allows us to use *manufactured solutions* for software esting, where we simply choose some function as solution, fit the corresponding ource term, and define boundary and initial conditions consistent with the ıosen solution. Such solutions will seldom fulfill the initial condition (3) so we eed to generalize this condition to $u_t = V(x)$.

.1 A slightly generalized model problem

Ve now address the following extended initial-boundary value problem for ne-dimensional wave phenomena:

$$
\begin{aligned}
u_{tt} &= c^2 u_{xx} + f(x,t), && x \in (0,L),\ t \in (0,T] \\
u(x,0) &= I(x), && x \in [0,L] \\
u_t(x,0) &= V(x), && x \in [0,L] \\
u(0,t) &= 0, && t > 0 \\
u(L,t) &= 0, && t > 0
\end{aligned}
$$

Sampling the PDE at (x_i, t_n) and using the same finite difference apı tions as above, yields

$$[D_t D_t u = c^2 D_x D_x + f]_i^n \,.$$

Writing this out and solving for the unknown u_i^{n+1} results in

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + C^2(u_{i+1}^n - 2u_i^n + u_{i-1}^n) + \Delta t^2 f_i^n \,.$$

The equation for the first time step must be rederived. The discretiz the initial condition $u_t = V(x)$ at $t = 0$ becomes

$$[D_{2t} u = V]_i^0 \quad \Rightarrow \quad u_i^{-1} = u_i^1 - 2\Delta t V_i,$$

which, when inserted in (23) for $n = 0$, gives the special formula

$$u_i^1 = u_i^0 - \Delta t V_i + \frac{1}{2} C^2 \left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right) + \frac{1}{2}\Delta t^2 f_i^n \,.$$

2.2 Using an analytical solution of physical significa

Many wave problems feature sinusoidal oscillations in time and spa example, the original PDE problem (1)-(5) allows a solution

$$u_{\mathrm{e}}(x,y,t)) = A \sin\left(\frac{\pi}{L}x\right) \cos\left(\frac{\pi}{L}ct\right) \,.$$

This u_{e} fulfills the PDE with $f = 0$, boundary conditions $u_{\mathrm{e}}(0,t) = u_{\mathrm{e}}(L$ as well as initial conditions $I(x) = A \sin\left(\frac{\pi}{L}x\right)$ and $V = 0$.

It is common to use such exact solutions of physical interest to verif mentations. However, the numerical solution u_i^n will only be an approx to $u_{\mathrm{e}}(x_i, t_n)$. We no have knowledge of the precise size of the error in this imation, and therefore we can never know if discrepancies between the co u_i^n and $u_{\mathrm{e}}(x_i, t_n)$ are caused by mathematical approximations or progr errors. In particular, if a plot of the computed solution u_i^n and the ex (25) looks similar, many are attempted to claim that the implementatio but there can still be serious programming errors although color plots lo

The only way to use exact physical solutions like (25) for serious and t verification is to run a series of finer and finer meshes, measure the int error in each mesh, and from this information estimate the convergence these rates are very close to 2, we have strong evidence that the implem works.

.3 Manufactured solution

)ne problem with the exact solution (25) is that it requires a simplification $' = 0, f = 0$) of the implemented problem (17)-(21). An advantage of using manufactured solution is that we can test all terms in the PDE problem. he idea of this approach is to set up some chosen solution and fit the source erm, boundary conditions, and initial conditions to be compatible with the iosen solution. Given that our boundary conditions in the implementation are $(0,t) = u(L,t) = 0$, we must choose a solution that fulfills these conditions.)ne example is

$$u_{\mathrm{e}}(x,t) = x(L-x)\sin t\,.$$

iserted in the PDE $u_{tt} = c^2 u_{xx} + f$ we get

$$-x(L-x)\sin t = -2\sin t + f \quad \Rightarrow f = (2 - x(L-x))\sin t\,.$$

he initial conditions become

$$\begin{aligned} u(x,0) &= I(x) = 0,\\ u_t(x,0) &= V(x) = (2 - x(L-x))\cos t\,. \end{aligned}$$

To verify the code, we run a series of refined meshes and compute the onvergence rates. Such tests rely on an assumption that some measure E of ie numerical error is related to the discretization parameters through

$$E = C_t \Delta t^r + C_x \Delta x^p,$$

here C_t, C_x, r, and p are constants. The constants r and p are known as the *onvergence rates* in time and space, respectively. From the accuracy in the finite ifference approximations, we expect $r = p = 2$. This is confirmed by truncation ror analysis and other types of analysis. By using an exact solution of the DE problem, we can empirically compute the error measure E on a sequence f refined meshes and see if the rates $r = p = 2$ are obtained. We will not be oncerned with estimating the constants C_t and C_x.

It is advantageous to introduce a single discretization parameter $h = \Delta t = \Delta x$ for some constant $\hat{c}$ (the idea is to keep $\Delta t^r/\Delta x^p$ constant). Since Δt and x are related through the Courant number, $\Delta t = C\Delta x/c$, we set $h = \Delta t$, and ien $\Delta x = hc/C$. Now the expression for the error measure is greatly simplified:

$$E = C_t \Delta t^r + C_x \Delta x^r = C_t h^r + \frac{C_x c}{C} h^r = \hat{C} h^r, \quad \hat{C} = C_t + \frac{C_x c}{C}\,.$$

We choose an initial discretization parameter h_0 and run experiments with ecreasing h: $h_i = 2^{-i} h_0$, $i = 1, 2, \ldots, m$. Halving h in each experiment is not ecessary, but a common choice. For each experiment we must record E and

h. A standard choice of error measure is the ℓ^2 or ℓ^∞ norm of the err function e_i^n:

$$\begin{aligned} E &= ||e_i^n||_{\ell^2} = \left(\Delta t \Delta x \sum_{n=0}^{N_t}\sum_{i=0}^{N_x} (e_i^n)^2\right)^{\frac{1}{2}}, \quad e_i^n = u_{\mathrm{e}}(x_i,t_n) - u_i^n,\\ E &= ||e_i^n||_{\ell^\infty} = \max_{i,n} |e_n^i|\,. \end{aligned}$$

In Python, one can compute $\sum_i (e_i^{n+1})^2$ at each time step and accumu value in some sum variable, say `e2_sum`. At the final time step one `sqrt(dt*dx*e2_sum)`. For the ℓ^∞ norm one must compare the maximu at a time level (`e.max()`) with the global maximum over the time `e_max = max(e_max, e.max())`.

An alternative error measure is to use a spatial norm at one time st e.g., the end time T:

$$\begin{aligned} E &= ||e_i^n||_{\ell^2} = \left(\Delta x \sum_{i=0}^{N_x} (e_i^n)^2\right)^{\frac{1}{2}}, \quad e_i^n = u_{\mathrm{e}}(x_i,t_n) - u_i^n,\\ E &= ||e_i^n||_{\ell^\infty} = \max_{0\le i\le N_x} |e_n^i|\,. \end{aligned}$$

Let E_i be the error measure in experiment (mesh) number i and l the corresponding discretization parameter (h). With the error model E_i we can estimate r by comparing two consecutive experiments: $E_{i+1} =$ and $E_i = \hat{C} h_i^r$. Dividing the two equations eliminates $\hat{C}$ and solving for

$$r_i = \frac{\ln E_{i+1}/E_i}{\ln h_{i+1}/h_i}, \quad i = 0, \ldots, m-1\,.$$

We should for the present discretization method observe that r_i approac i increases.

2.4 Constructing an exact solution of the discrete tions

With a manufactured or known analytical solution, as outlined above, estimate convergence rates and see if they have the correct asymptotic b Experience shows that this is a quite good verification technique in tha common bugs will destroy the convergence rates. A significantly bet would be to check that the numerical solution is exactly what it sh This will in general require knowledge of the numerical error, which w have. However, it is possible to look for solutions where we can show t numerical error vanishes, i.e., the solution of the PDE problem is also a of the discrete equations. This property often arises if the exact solut

ower-order polynomial. (Truncation error analysis leads to error measures that nvolve derivatives of the exact solution. In the present problem, the truncation rror involves 4th-order derivatives of u in space and time. Choosing u as a olynomial of degree three or less will therefore lead to vanishing error.)

We shall now illustrate the construction of an exact solution of the PDE roblem and the discrete equations. Our choice of manufactured solution is uadratic in space and linear in time. More specifically, we set

$$u_{\mathrm{e}}(x,t) = x(L-x)(1+\frac{1}{2}t), \tag{30}$$

hich by insertion in the PDE leads to $f(x,t) = 2(1+t)c^2$. This u_{e} fulfills the oundary conditions $u = 0$ and demands $I(x) = x(L-x)$ and $V(x) = \frac{1}{2}x(L-x)$.

To realize that the chosen u_{e} is that it is also an exact solution of the discrete quations, we first establish the results

$$[D_tD_t t^2]^n = \frac{t_{n+1}^2 - 2t_n^2 + t_{n-1}^2}{\Delta t^2} = (n+1)^2 - n^2 + (n-1)^2 = 2, \tag{31}$$

$$[D_tD_t t]^n = \frac{t_{n+1} - 2t_n + t_{n-1}}{\Delta t^2} = \frac{((n+1) - n + (n-1))\Delta t}{\Delta t^2} = 0\,. \tag{32}$$

ence,

$$[D_tD_t u_{\mathrm{e}}]_i^n = x_i(L-x_i)[D_tD_t(1+\frac{1}{2}t)]^n = x_i(L-x_i)\frac{1}{2}[D_tD_t t]^n = 0,$$

nd

$$\begin{aligned}[D_xD_x u_{\mathrm{e}}]_i^n &= (1+\frac{1}{2}t_n)[D_xD_x(xL-x^2)]_i = (1+\frac{1}{2}t_n)[LD_xD_x x - D_xD_x x^2]_i \\ &= -2(1+\frac{1}{2}t_n)\,.\end{aligned}$$

ow, $f_i^n = 2(1+\frac{1}{2}t_n)c^2$ and we get

$$[D_tD_t u_{\mathrm{e}} - c^2 D_xD_x u_{\mathrm{e}} - f]_i^n = 0 - c^2(-1)2(1+\frac{1}{2}t_n + 2(1+\frac{1}{2}t_n)c^2 = 0\,.$$

Moreover, $u_{\mathrm{e}}(x_i,0) = I(x_i)$, $\partial u_{\mathrm{e}}/\partial t = V(x_i)$ at $t = 0$, and $u_{\mathrm{e}}(x_0,t) = {}_{\mathrm{e}}(x_{N_x},0) = 0$. Also the modified scheme for the first time step is fulfilled by ${}_{\mathrm{e}}(x_i,t_n)$.

Therefore, the exact solution $u_{\mathrm{e}}(x,t) = x(L-x)(1+t/2)$ of the PDE problem also an exact solution of the discrete problem. We can use this result to check hat the computed u_i^n vales from an implementation equals $u_{\mathrm{e}}(x_i,t_n)$ within achine precision, *regardless of the mesh spacings* Δx and Δt! Nevertheless, here might be stability restrictions on Δx and Δt, so the test can only be run or a mesh that is compatible with the stability criterion (which in the present ase is $C \leq 1$, to be derived later).

Notice.

A product of quadratic or linear expressions in the various indepen variables, as shown above, will often fulfill both the continuous and dis PDE problem and can therefore be very useful solutions for veri implementations. However, for 1D wave equations of the type $u_t =$ we shall see that there is always another much more powerful w generating exact solutions (just set $C = 1$).

3 Implementation

This section present the complete computational algorithm, its implement Python code, animation of the solution, and verification of the impleme

A real implementation of the basic computational algorithm from Sect and 1.6 can be encapsulated in a function, taking all the input data problem as arguments. The physical input data consists of c, $I(x)$, $V(x)$ L, and T. The numerical input is the mesh parameters Δt and Δx.

Instead of specifying Δt *and* Δx, we can specify one of them and the number C instead, since having explicit control of the Courant nu convenient when investigating the numerical method. Many find it na prescribe the resolution of the spatial grid and set N_x. The solver f can then compute $\Delta t = CL/(cN_x)$. However, for comparing $u(x,t)$ cu functions of x) for various Courant numbers, especially in animations it is more convenient to keep Δt fixed for all C and let Δx vary acco $\Delta x = c\Delta t/C$. (With Δt fixed, all frames correspond to the same tim plotting curves with different spatial resolution is trivial.)

The solution at all spatial points at a new time level is stored in a `u` (of length N_x+1). We need to decide what do to with this soluti visualize the curve, analyze the values, or write the array to file for l The decision what to do is left to the user in a suppled function

```
def user_action(u, x, t, n):
```

where `u` is the solution at the spatial points `x` at time `t[n]`.

3.1 Making a solver function

A first attempt at a solver function is listed below.

```
from numpy import *

def solver(I, V, f, c, L, dt, C, T, user_action=None):
    """Solve u_tt=c^2*u_xx + f on (0,L)x(0,T]."""
    Nt = int(round(T/dt))
    t = linspace(0, Nt*dt, Nt+1)   # Mesh points in time
    dx = dt*c/float(C)
```

```
    Nx = int(round(L/dx))
    x = linspace(0, L, Nx+1)       # Mesh points in space
    C2 = C**2                      # Help variable in the scheme
    if f is None or f == 0 :
        f = lambda x, t: 0
    if V is None or V == 0:
        V = lambda x: 0

    u   = zeros(Nx+1)   # Solution array at new time level
    u_1 = zeros(Nx+1)   # Solution at 1 time level back
    u_2 = zeros(Nx+1)   # Solution at 2 time levels back

    import time;  t0 = time.clock()  # for measuring CPU time

    # Load initial condition into u_1
    for i in range(0,Nx+1):
        u_1[i] = I(x[i])

    if user_action is not None:
        user_action(u_1, x, t, 0)

    # Special formula for first time step
    n = 0
    for i in range(1, Nx):
        u[i] = u_1[i] + dt*V(x[i]) + \
               0.5*C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1]) + \
               0.5*dt**2*f(x[i], t[n])
    u[0] = 0;  u[Nx] = 0

    if user_action is not None:
        user_action(u, x, t, 1)

    # Switch variables before next step
    u_2[:], u_1[:] = u_1, u

    for n in range(1, Nt):
        # Update all inner points at time t[n+1]
        for i in range(1, Nx):
            u[i] = - u_2[i] + 2*u_1[i] + \
                     C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1]) + \
                     dt**2*f(x[i], t[n])

        # Insert boundary conditions
        u[0] = 0;  u[Nx] = 0
        if user_action is not None:
            if user_action(u, x, t, n+1):
                break

        # Switch variables before next step
        u_2[:], u_1[:] = u_1, u

    cpu_time = t0 - time.clock()
    return u, x, t, cpu_time
```

.2 Verification: exact quadratic solution

We use the test problem derived in Section 2.1 for verification. Here is a function realizing this verification as a nose test:


```
import nose.tools as nt

def test_quadratic():
    """Check that u(x,t)=x(L-x)(1+t/2) is exactly reproduced."""
    def u_exact(x, t):
        return x*(L-x)*(1 + 0.5*t)

    def I(x):
        return u_exact(x, 0)

    def V(x):
        return 0.5*u_exact(x, 0)

    def f(x, t):
        return 2*(1 + 0.5*t)*c**2

    L = 2.5
    c = 1.5
    C = 0.75
    Nx = 3  # Very coarse mesh for this exact test
    dt = C*(L/Nx)/c
    T = 18

    u, x, t, cpu = solver(I, V, f, c, L, dt, C, T)
    u_e = u_exact(x, t[-1])
    diff = abs(u - u_e).max()
    nt.assert_almost_equal(diff, 0, places=14)
```

3.3 Visualization: animating the solution

Now that we have verified the implementation it is time to do a real comp where we also display the evolution of the waves on the screen.

Visualization via SciTools. The following `viz` function defines a user callback function for plotting the solution at each time level:

```
def viz(I, V, f, c, L, dt, C, T, umin, umax, animate=True):
    """Run solver and visualize u at each time level."""
    import scitools.std as plt
    import time, glob, os

    def plot_u(u, x, t, n):
        """user_action function for solver."""
        plt.plot(x, u, 'r-',
                 xlabel='x', ylabel='u',
                 axis=[0, L, umin, umax],
                 title='t=%f' % t[n], show=True)
        # Let the initial condition stay on the screen for 2
        # seconds, else insert a pause of 0.2 s between each plot
        time.sleep(2) if t[n] == 0 else time.sleep(0.2)
        plt.savefig('frame_%04d.png' % n)  # for movie making

    # Clean up old movie frames
    for filename in glob.glob('frame_*.png'):
        os.remove(filename)
```

```
    user_action = plot_u if animate else None
    u, x, t, cpu = solver(I, V, f, c, L, dt, C, T, user_action)

    # Make movie files
    fps = 4  # Frames per second
    plt.movie('frame_*.png', encoder='html', fps=fps,
              output_file='movie.html')
    codec2ext = dict(flv='flv', libx264='mp4', libvpx='webm',
                     libtheora='ogg')
    filespec = 'frame_%04d.png'
    movie_program = 'avconv'  # or 'ffmpeg'
    for codec in codec2ext:
        ext = codec2ext[codec]
        cmd = '%(movie_program)s -r %(fps)d -i %(filespec)s '\
              '-vcodec %(codec)s movie.%(ext)s' % vars()
        os.system(cmd)
```

function inside another function, like `plot_u` in the above code segment, has ccess to *and remembers* all the local variables in the surrounding code inside ıe `viz` function (!). This is known in computer science as a *closure* and is ery convenient to program with. For example, the `plt` and `time` modules efined outside `plot_u` are accessible for `plot_u` when the function is called (as `ser_action`) in the `solver` function. Some may think, however, that a class ıstead of a closure is a cleaner and easier-to-understand implementation of the ser action function, see Section 8.

Making movie files. Several hardcopies of the animation are made from ıe `frame_*.png` files. We use the `avconv` (or `ffmpeg`) programs to combine ıdividual plot files to movies in modern formats: Flash, MP4, Webm, and)gg. A typical `avconv` (or `ffmpeg`) command for creating a movie file in Ogg ›rmat with 4 frames per second built from a collection of plot files with names enerated by `frame_%04d.png`, look like

```
erminal> avconv -r 4 -i frame_%04d.png -c:v libtheora movie.ogg
```

he different formats require different video encoders (`-c:v`) to be installed: lash applies `flv`, WebM applies `libvpx`, and MP4 applies `libx264`:

```
erminal> avconv -r 4 -i frame_%04d.png -c:v flv movie.flv
erminal> avconv -r 4 -i frame_%04d.png -c:v libvpx movie.webm
erminal> avconv -r 4 -i frame_%04d.png -c:v libx264 movie.mp4
```

Players like `vlc`, `mplayer`, `gxine`, and `totem` can be used to play these movie les.

Note that padding the frame counter with zeros in the `frame_*.png` files, s specified by the `%04d` format, is essential so that the wildcard notation `rame_*.png` expands to the correct set of files.

The `plt.movie` function also creates a `movie.html` file with a movi for displaying the `frame_*.png` files in a web browser. This movie playe generated from the command line too

```
Terminal> scitools movie encoder=html output_file=movie.html \
          fps=4 frame_*.png
```

Skipping frames for animation speed. Sometimes the time step and T is large, leading to an inconveniently large number of plot files an animation on the screen. The solution to such a problem is to decide or number of frames in the animation, `num_frames`, and plot the solution every `every` frame. The total number of time levels (i.e., maximum number of frames) is the length of `t`, `t.size`, and if we want `num_fra` need to plot every `t.size/num_frames` frame:

```
every = int(t.size/float(num_frames))
if n % every == 0 or n == t.size-1:
    st.plot(x, u, 'r-', ...)
```

The initial condition (`n=0`) is natural to include, and as `n % every =` very seldom be true for the very final frame, we also ensure that `n == t.` and hence the final frame is included.

A simple choice of numbers may illustrate the formulas: say we h frames in total (`t.size`) and we allow only 60 frames to be plotted. T need to plot every 801/60 frame, which with integer division yields 13 a Using the mod function, `n % every`, this operation is zero every time `n` divided by 13 without a remainder. That is, the `if` test is true when `n` $0, 13, 26, 39, ..., 780, 801$. The associated code is included in the `plot_u` in the file `wave1D_u0v.py`[3].

Visualization via Matplotlib. The previous code based on the `plot` i from `scitools.std` can be run with Matplotlib as the visualization b but if one desires to program directly with Matplotlib, quite different needed. Matplotlib's interactive mode must be turned on:

```
import matplotlib.pyplot as plt
plt.ion()  # interactive mode on
```

The most commonly used animation technique with Matplotlib is to up data in the plot at each time level:

```
# Make a first plot
lines = plt.plot(t, u)
# call plt.axis, plt.xlabel, plt.ylabel, etc. as desired
```

[3] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_u0v.py`

```
# At later time levels
lines[0].set_ydata(u)
plt.legend('t=%g' % t[n])
plt.draw()  # make updated plot
plt.savefig(...)
```

An alternative is to rebuild the plot at every time level:

```
plt.clf()        # delete any previous curve(s)
plt.axis([...])
plt.plot(t, u)
# plt.xlabel, plt.legend and other decorations
plt.draw()
plt.savefig(...)
```

Many prefer to work with figure and axis objects as in MATLAB:

```
fig = plt.figure()
...
fig.clf()
ax = fig.gca()
ax.axis(...)
ax.plot(t, u)
# ax.set_xlabel, ax.legend and other decorations
plt.draw()
fig.savefig(...)
```

.4 Running a case

The first demo of our 1D wave equation solver concerns vibrations of a string that is initially deformed to a triangular shape, like when picking a guitar string:

$$I(x) = \begin{cases} ax/x_0, & x < x_0, \\ a(L-x)/(L-x_0), & \text{otherwise} \end{cases} \tag{33}$$

We choose $L = 75$ cm, $x_0 = 0.8L$, $a = 5$ mm, and a time frequency $\nu = 440$ Hz. The relation between the wave speed c and ν is $c = \nu\lambda$, where λ is the wavelength, taken as $2L$ because the longest wave on the string form half a wavelength. There is no external force, so $f = 0$, and the string is at rest initially so that $V = 0$.

Regarding numerical parameters, we need to specify a Δt. Sometimes it is more natural to think of a spatial resolution instead of a time step. A natural semi-coarse spatial resolution in the present problem is $N_x = 50$. We can then choose the associated Δt (as required by the `viz` and `solver` functions) as the stability limit: $\Delta t = L/(N_x c)$. This is the Δt to be specified, but notice that if $C < 1$, the actual Δx computed in `solver` gets larger than L/N_x: $\Delta x = c\Delta t/C = L/(N_x C)$. (The reason is that we fix Δt and adjust Δx, so if C gets smaller, the code implements this effect in terms of a larger Δx.)

A function for setting the physical and numerical parameters and calling `viz` in this application goes as follows:


```
def guitar(C):
    """Triangular wave (pulled guitar string)."""
    L = 0.75
    x0 = 0.8*L
    a = 0.005
    freq = 440
    wavelength = 2*L
    c = freq*wavelength
    omega = 2*pi*freq
    num_periods = 1
    T = 2*pi/omega*num_periods
    # Choose dt the same as the stability limit for Nx=50
    dt = L/50./c

    def I(x):
        return a*x/x0 if x < x0 else a/(L-x0)*(L-x)

    umin = -1.2*a;  umax = -umin
    cpu = viz(I, 0, 0, c, L, dt, C, T, umin, umax, animate=True)
```

The associated program has the name `wave1D_u0.py`[4]. Run the progr watch the movie of the vibrating string[5].

3.5 The benefits of scaling

The previous example demonstrated that quite some work is needed tablishing relevant physical parameters for a case. By *scaling* the mathe problem we can often reduce the need to estimate physical parameters cally. A scaling consists of introducing new independent and dependent v with the aim that the absolute value of these vary between 0 and 1:

$$\bar{x} = \frac{x}{L}, \quad \bar{t} = \frac{c}{L}t, \quad \bar{u} = \frac{u}{a}.$$

Replacing old by new variables in the PDE, using $f = 0$, and dropping t results in the *scaled equation* $u_{tt} = u_{xx}$. This equation has no physical pa (!).

If we have a program implemented for the physical wave equati dimensions, we can obtain the dimensionless, scaled version by settin The initial condition corresponds to (185), but with setting $a = 1$, $L =$ $x_0 \in [0, 1]$. This means that we only need to decide on the x_0 value as a of unity, because the scaled problem corresponds to setting all other par to unity! In the code we can just set `a=c=L=1`, `x0=0.8`, and there is no calculate with wavelengths and frequencies to estimate c.

The only non-trivial parameter to estimate in the scaled problem is t end time of the simulation, or more precisely, how it relates to periods in solutions in time, since we often want to express the end time as a number of periods. Suppose as u behaves as $\sin(\omega t)$ in time in variab dimension. The corresponding period is $P = 2\pi/\omega$. The frequency ω is re

[4] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_u0.py`
[5] `http://tinyurl.com/opdfafk/pub/mov-wave/guitar_C0.8/index.html`

ıe wavelength λ of the waves through the relations $\omega = kc$ and $k = 2\pi/\lambda$, giving
$= 2\pi c/\lambda$ and $P = \lambda/c$. It remains to estimate λ. With $u(x,t) = F(x)\sin\omega t$
e find from $u_{tt} = c^2 u_{xx}$ that $c^2F'' + \omega^2 F = 0$, and the boundary conditions
emand $F(0) = F(L) = 0$. The solution is $F(x) = \sin(x\pi/L)$, which has
avelength $\lambda = 2\pi/(\pi/L) = 2L$. One period is therefore given by $P = 2L/c$.
he dimensionless period is $\bar{P} = Pc/L = 2$.

: Vectorization

he computational algorithm for solving the wave equation visits one mesh
oint at a time and evaluates a formula for the new value u_i^{n+1} at that point.
echnically, this is implemented by a loop over array elements in a program.
uch loops may run slowly in Python (and similar interpreted languages such as
, and MATLAB). One technique for speeding up loops is to perform operations
ı entire arrays instead of working with one element at a time. This is referred
› as *vectorization*, *vector computing*, or *array computing*. Operations on whole
rrays are possible if the computations involving each element is independent of
ach other and therefore can, at least in principle, be performed simultaneously.
ectorization not only speeds up the code on serial computers, but it also makes
easy to exploit parallel computing.

.1 Operations on slices of arrays

fficient computing with `numpy` arrays demands that we avoid loops and compute
ith entire arrays at once (or at least large portions of them). Consider this
alculation of differences $d_i = u_{i+1} - u_i$:

```
ı = u.size
for i in range(0, n-1):
    d[i] = u[i+1] - u[i]
```

ll the differences here are independent of each other. The computation of `d` can
ıerefore alternatively be done by subtracting the array $(u_0, u_1, \ldots, u_{n-1})$ from
ıe array where the elements are shifted one index upwards: $(u_1, u_2, \ldots, u_n)$,
ee Figure 3. The former subset of the array can be expressed by `u[0:n-1]`,
`[0:-1]`, or just `u[:-1]`, meaning from index 0 up to, but not including, the
ıst element (`-1`). The latter subset is obtained by `u[1:n]` or `u[1:]`, meaning
om index 1 and the rest of the array. The computation of `d` can now be done
ithout an explicit Python loop:

```
d = u[1:] - u[:-1]
```

r with explicit limits if desired:

```
d = u[1:n] - u[0:n-1]
```


Indices with a colon, going from an index to (but not including) anothe
are called *slices*. With `numpy` arrays, the computations are still done b
but in efficient, compiled, highly optimized code in C or Fortran. Suc
operations can also easily be distributed among many processors on
computers. We say that the *scalar code* above, working on an element (a
at a time, has been replaced by an equivalent *vectorized code*. The pr
vectorizing code is called *vectorization*.

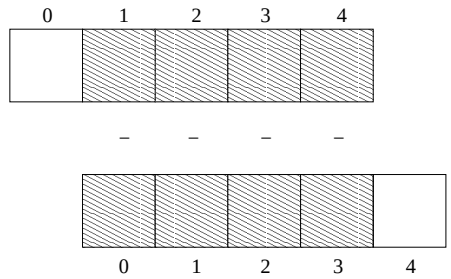


Figure 3: Illustration of subtracting two slices of two arrays.

Test the understanding.

Newcomers to vectorization are encouraged to choose a small array u
with five elements, and simulate with pen and paper both the loop ve
and the vectorized version.

Finite difference schemes basically contains differences between array e
with shifted indices. Consider the updating formula

```
for i in range(1, n-1):
    u2[i] = u[i-1] - 2*u[i] + u[i+1]
```

The vectorization consists of replacing the loop by arithmetics on slices c
of length `n-2`:

```
u2 = u[:-2] - 2*u[1:-1] + u[2:]
u2 = u[0:n-2] - 2*u[1:n-1] + u[2:n]   # alternative
```

Note that `u2` here gets length `n-2`. If `u2` is already an array of length `n`
want to use the formula to update all the "inner" elements of `u2`, as we w
solving a 1D wave equation, we can write

```
u2[1:-1]  = u[:-2] - 2*u[1:-1] + u[2:]
u2[1:n-1] = u[0:n-2] - 2*u[1:n-1] + u[2:n]   # alternative
```

Pen and paper calculations with a small array will demonstrate what is
going on. The expression on the right-hand side are done in the followir

nvolving temporary arrays with intermediate results, since we can only work ith two arrays at a time in arithmetic expressions:

```
emp1 = 2*u[1:-1]
emp2 = u[0:-2] - temp1
emp3 = temp2 + u[2:]
u2[1:-1] = temp3
```

We can extend the previous example to a formula with an additional term omputed by calling a function:

```
def f(x):
    return x**2 + 1

for i in range(1, n-1):
    u2[i] = u[i-1] - 2*u[i] + u[i+1] + f(x[i])
```

ssuming `u2`, `u`, and `x` all have length `n`, the vectorized version becomes

```
u2[1:-1] = u[:-2] - 2*u[1:-1] + u[2:] + f(x[1:-1])
```

.2 Finite difference schemes expressed as slices

We now have the necessary tools to vectorize the algorithm for the wave equation. here are three loops: one for the initial condition, one for the first time step, nd finally the loop that is repeated for all subsequent time levels. Since only he latter is repeated a potentially large number of times, we limit the efforts of ectorizing the code to this loop:

```
for i in range(1, Nx):
    u[i] = 2*u_1[i] - u_2[i] + \
           C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1])
```

he vectorized version becomes

```
u[1:-1] = - u_2[1:-1] + 2*u_1[1:-1] + \
          C2*(u_1[:-2] - 2*u_1[1:-1] + u_1[2:])
```

```
u[1:Nx] = 2*u_1[1:Nx]- u_2[1:Nx] + \
          C2*(u_1[0:Nx-1] - 2*u_1[1:Nx] + u_1[2:Nx+1])
```

The program `wave1D_u0v.py`[6] contains a new version of the function `solver` here both the scalar and the vectorized loops are included (the argument `ersion` is set to `scalar` or `vectorized`, respectively).

[6] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_u0v.py`

4.3 Verification

We may reuse the quadratic solution $u_e(x,t) = x(L-x)(1+\frac{1}{2}t)$ for verify the vectorized code. A nose test can now test both the scalar and the ve version. Moreover, we may use a `user_action` function that compa computed and exact solution at each time level and performs a test:

```
def test_quadratic():
    """
    Check the scalar and vectorized versions work for
    a quadratic u(x,t)=x(L-x)(1+t/2) that is exactly reproduced.
    """
    # The following function must work for x as array or scalar
    u_exact = lambda x, t: x*(L - x)*(1 + 0.5*t)
    I = lambda x: u_exact(x, 0)
    V = lambda x: 0.5*u_exact(x, 0)
    # f is a scalar (zeros_like(x) works for scalar x too)
    f = lambda x, t: zeros_like(x) + 2*c**2*(1 + 0.5*t)

    L = 2.5
    c = 1.5
    C = 0.75
    Nx = 3  # Very coarse mesh for this exact test
    dt = C*(L/Nx)/c
    T = 18

    def assert_no_error(u, x, t, n):
        u_e = u_exact(x, t[n])
        diff = abs(u - u_e).max()
        nt.assert_almost_equal(diff, 0, places=13)

    solver(I, V, f, c, L, dt, C, T,
           user_action=assert_no_error, version='scalar')
    solver(I, V, f, c, L, dt, C, T,
           user_action=assert_no_error, version='vectorized')
```

Lambda functions.

The code segment above demonstrates how to achieve very compact with the use of lambda functions for the various input parameters require a Python function. In essence,

```
f = lambda x, t: L*(x-t)**2
```

is equivalent to

```
def f(x, t):
    return L(x-t)**2
```

Note that lambda functions can just contain a single expression an statements.

One advantage with lambda functions is that they can be used directly in calls:

```
solver(I=lambda x: sin(pi*x/L), V=0, f=0, ...)
```

.4 Efficiency measurements

unning the `wave1D_u0v.py` code with the previous string vibration exam-le for $N_x = 50, 100, 200, 400, 800$, and measuring the CPU time (see the `un_efficiency_experiments` function), shows that the vectorized code runs ubstantially faster: the scalar code uses approximately a factor $N_x/5$ more me!

Exercises

Exercise 1: Simulate a standing wave

he purpose of this exercise is to simulate standing waves on $[0, L]$ and illustrate ie error in the simulation. Standing waves arise from an initial condition

$$u(x, 0) = A \sin\left(\frac{\pi}{L} mx\right),$$

here m is an integer and A is a freely chosen amplitude. The corresponding xact solution can be computed and reads

$$u_{\mathrm{e}}(x, t) = A \sin\left(\frac{\pi}{L} mx\right) \cos\left(\frac{\pi}{L} mct\right).$$

) Explain that for a function $\sin kx \cos \omega t$ the wave length in space is $\lambda = 2\pi/k$ nd the period in time is $P = 2\pi/\omega$. Use these expressions to find the wave ngth in space and period in time of u_{e} above.

) Import the `solver` function `wave1D_u0.py` into a new file where the `viz` nction is reimplemented such that it plots either the numerical *and* the exact olution, *or* the error.

) Make animations where you illustrate how the error $e_i^n = u_{\mathrm{e}}(x_i, t_n) - u_i^n$ evelops and increases in time. Also make animations of u and u_{e} simultaneously.

lint 1. Quite long time simulations are needed in order to display significant iscrepancies between the numerical and exact solution.

Hint 2. A possible set of parameters is $L = 12$, $m = 9$, $c = 2$, $A = 1$, l $C = 0.8$. The error mesh function e^n can be simulated for 10 period 20-30 periods are needed to show significant differences between the cu the numerical and exact solution.
Filename: `wave_standing.py`.

Remarks. The important parameters for numerical quality are C a where $C = c\Delta t/\Delta x$ is the Courant number and k is defined above proportional to how many mesh points we have per wave length in sp Section 10.4 for explanation).

Exercise 2: Add storage of solution in a user action fu

Extend the `plot_u` function in the file `wave1D_u0.py` to also store the s `u` in a list. To this end, declare `all_u` as an empty list in the `viz` f outside `plot_u`, and perform an append operation inside the `plot_u` f Note that a function, like `plot_u`, inside another function, like `viz`, ren all local variables in `viz` function, including `all_u`, even when `plot_u` (as `user_action`) in the `solver` function. Test both `all_u.append(` `all_u.append(u.copy())`. Why does one of these constructions fail the solution correctly? Let the `viz` function return the `all_u` list conver two-dimensional `numpy` array. Filename: `wave1D_u0_s_store.py`.

Exercise 3: Use a class for the user action function

Redo Exercise 2 using a class for the user action function. That is, defin `Action` where the `all_u` list is an attribute, and implement the user acti tion as a method (the special method `__call__` is a natural choice). T versions avoids that the user action function depends on parameters defi side the function (such as `all_u` in Exercise 2). Filename: `wave1D_u0_`

Exercise 4: Compare several Courant numbers in one

The goal of this exercise is to make movies where several curves, corres to different Courant numbers, are visualized. Import the `solver` functi the `wave1D_u0_s` movie in a new file `wave_compare.py`. Reimplement function such that it can take a list of `C` values as argument and create with solutions corresponding to the given `C` values. The `plot_u` functi be changed to store the solution in an array (see Exercise 2 or 3 for `solver` must be computed for each value of the Courant number, an one must run through each time step and plot all the spatial solution c one figure and store it in a file.

The challenge in such a visualization is to ensure that the curves in corresponds to the same time point. The easiest remedy is to keep the t space resolution constant and change the wave velocity c to change the number. Filename: `wave_numerics_comparison.py`.

Project 5: Calculus with 1D mesh functions

This project explores integration and differentiation of mesh functions, both with scalar and vectorized implementations. We are given a mesh function f_i on a spatial one-dimensional mesh $x_i = i\Delta x$, $i = 0, \ldots, N_x$, over the interval $[a, b]$.

) Define the discrete derivative of f_i by using centered differences at internal mesh points and one-sided differences at the end points. Implement a scalar version of the computation in a Python function and supply a nose test for the linear case $f(x) = 4x - 2.5$ where the discrete derivative should be exact.

) Vectorize the implementation of the discrete derivative. Extend the nose test to check the validity of the implementation.

) To compute the discrete integral F_i of f_i, we assume that the mesh function f_i varies linearly between the mesh points. Let $f(x)$ be such a linear interpolant of f_i. We then have

$$F_i = \int_{x_0}^{x_i} f(x)dx\,.$$

The exact integral of a piecewise linear function $f(x)$ is given by the Trapezoidal rule. S how that if F_i is already computed, we can find F_{i+1} from

$$F_{i+1} = F_i + \frac{1}{2}(f_i + f_{i+1})\Delta x\,.$$

Make a function for a scalar implementation of the discrete integral as a mesh function. That is, the function should return F_i for $i = 0, \ldots, N_x$. For a nose test one can use the fact that the above defined discrete integral of a linear function (say $f(x) = 4x - 2.5$) is exact.

) Vectorize the implementation of the discrete integral. Extend the nose test to check the validity of the implementation.

Hint. Interpret the recursive formula for F_{i+1} as a sum. Make an array with each element of the sum and use the "cumsum" (`numpy.cumsum`) operation to compute the accumulative sum: `numpy.cumsum([1,3,5])` is `[1,4,9]`.

) Create a class `MeshCalculus` that can integrate and differentiate mesh functions. The class can just define some methods that call the previously implemented Python functions. Here is an example on the usage:

```
import numpy as np
calc = MeshCalculus(vectorized=True)
x = np.linspace(0, 1, 11)        # mesh
f = np.exp(x)                    # mesh function
df = calc.differentiate(f, x)    # discrete derivative
F = calc.integrate(f, x)         # discrete anti-derivative
```

Filename: `mesh_calculus_1D.py`.

6 Generalization: reflecting boundaries

The boundary condition $u = 0$ makes u change sign at the boundary, the condition $u_x = 0$ perfectly reflects the wave, see a web page[7] or a file[8] for demonstration. Our next task is to explain how to implement boundary condition $u_x = 0$, which is more complicated to express numerically and also to implement than a given value of u. We shall present two methods for implementing $u_x = 0$ in a finite difference scheme, one based on deriving a modified stencil at the boundary, and another one based on extending the mesh with ghost cells and ghost points.

6.1 Neumann boundary condition

When a wave hits a boundary and is to be reflected back, one applies the condition

$$\frac{\partial u}{\partial n} \equiv \boldsymbol{n}\cdot\nabla u = 0\,.$$

The derivative $\partial/\partial n$ is in the outward normal direction from a general boundary. For a 1D domain $[0, L]$, we have that

$$\left.\frac{\partial}{\partial n}\right|_{x=L} = \frac{\partial}{\partial x}, \quad \left.\frac{\partial}{\partial n}\right|_{x=0} = -\frac{\partial}{\partial x}\,.$$

Boundary condition terminology.

Boundary conditions that specify the value of $\partial u/\partial n$, or shorter u_n, are known as Neumann[a] conditions, while Dirichlet conditions[b] refer to specifications of u. When the values are zero ($\partial u/\partial n = 0$ or $u = 0$) we say that about *homogeneous* Neumann or Dirichlet conditions.

[a] http://en.wikipedia.org/wiki/Neumann_boundary_condition
[b] http://en.wikipedia.org/wiki/Dirichlet_conditions

6.2 Discretization of derivatives at the boundary

How can we incorporate the condition (34) in the finite difference scheme we have used central differences in all the other approximations to derivatives in the scheme, it is tempting to implement (34) at $x = 0$ and $t = t_n$ by a difference

$$\frac{u^n_{-1} - u^n_1}{2\Delta x} = 0\,.$$

[7] http://tinyurl.com/opdfafk/pub/mov-wave/demo_BC_gaussian/index.html
[8] http://tinyurl.com/opdfafk/pub/mov-wave/demo_BC_gaussian/movie.flv

he problem is that u^n_{-1} is not a u value that is being computed since the point outside the mesh. However, if we combine (35) with the scheme for $i = 0$,

$$u^{n+1}_i = -u^{n-1}_i + 2u^n_i + C^2\left(u^n_{i+1} - 2u^n_i + u^n_{i-1}\right), \tag{36}$$

e can eliminate the fictitious value u^n_{-1}. We see that $u^n_{-1} = u^n_1$ from (35), which an be used in (36) to arrive at a modified scheme for the boundary point u^{n+1}_0:

$$u^{n+1}_i = -u^{n-1}_i + 2u^n_i + 2C^2\left(u^n_{i+1} - u^n_i\right), \quad i = 0\,. \tag{37}$$

igure 4 visualizes this equation for computing u^3_0 in terms of u^2_0, u^1_0, and u^2_1.

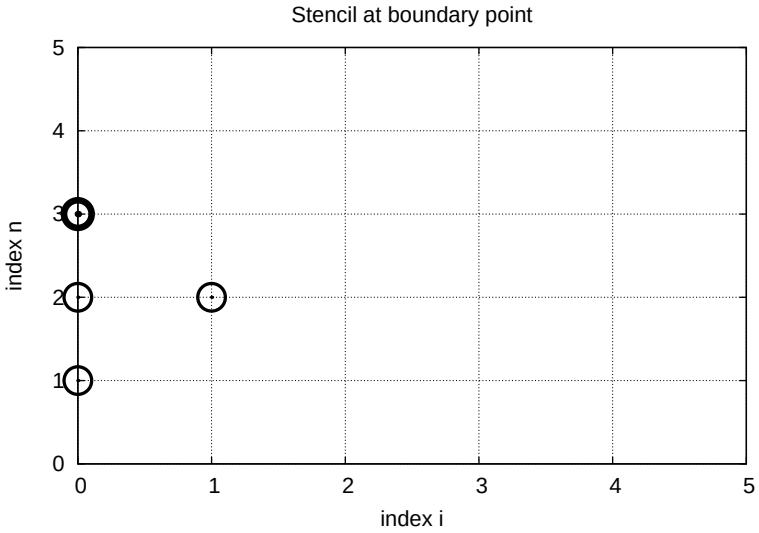


Figure 4: Modified stencil at a boundary with a Neumann condition.

Similarly, (34) applied at $x = L$ is discretized by a central difference

$$\frac{u^n_{N_x+1} - u^n_{N_x-1}}{2\Delta x} = 0\,. \tag{38}$$

ombined with the scheme for $i = N_x$ we get a modified scheme for the boundary alue $u^{n+1}_{N_x}$:

$$u^{n+1}_i = -u^{n-1}_i + 2u^n_i + 2C^2\left(u^n_{i-1} - u^n_i\right), \quad i = N_x\,. \tag{39}$$

The modification of the scheme at the boundary is also required for the pecial formula for the first time step. How the stencil moves through the mesh nd is modified at the boundary can be illustrated by an animation in a web age[9] or a movie file[10].

[9] http://tinyurl.com/opdfafk/pub/mov-wave/wave1D_PDE_Neumann_stencil_gpl/index.html
[10] http://tinyurl.com/opdfafk/pub/mov-wave/wave1D_PDE_Neumann_stencil_gpl/movie.ogg

6.3 Implementation of Neumann conditions

The implementation of the special formulas for the boundary points can from using the general formula for the interior points also at the bou but replacing u^n_{i-1} by u^n_{i+1} when computing u^{n+1}_i for $i = 0$ and u^n_{i+1} by $i = N_x$. This is achieved by just replacing the index $i-1$ by $i+1$ for i $i+1$ by $i-1$ for $i = N_x$. In a program, we introduce variables to hold t of the offset indices: `im1` for `i-1` and `ip1` for `i+1`. It is now just a ma defining `im1` and `ip1` properly for the internal points and the boundary The coding for the latter reads

```
i = 0
ip1 = i+1
im1 = ip1  # i-1 -> i+1
u[i] = u_1[i] + C2*(u_1[im1] - 2*u_1[i] + u_1[ip1])

i = Nx
im1 = i-1
ip1 = im1  # i+1 -> i-1
u[i] = u_1[i] + C2*(u_1[im1] - 2*u_1[i] + u_1[ip1])
```

We can in fact create one loop over both the internal and boundary and use only one updating formula:

```
for i in range(0, Nx+1):
    ip1 = i+1 if i < Nx else i-1
    im1 = i-1 if i > 0  else i+1
    u[i] = u_1[i] + C2*(u_1[im1] - 2*u_1[i] + u_1[ip1])
```

The program `wave1D_n0.py`[11] contains a complete implementatio 1D wave equation with boundary conditions $u_x = 0$ at $x = 0$ and $x = I$

It would be nice to modify the `test_quadratic` test case from the `wav` with Dirichlet conditions, described in Section 4.3. However, the Neuma ditions requires the polynomial variation in x directory to be of third which causes challenging problems with designing a test where the nu solution is known exactly. Exercise 10 outlines ideas and code for this The only test in `wave1D_n0.py` is to start with a plug wave at rest and the initial condition is reached again perfectly after one period of m $C = 1$.

6.4 Index set notation

We shall introduce a special notation for index sets, consisting of wr $i \in \mathcal{I}_x$, instead of $i = 0, \ldots, N_x$. Obviously, $\mathcal{I}_x$ must be the set $\mathcal{I}_x = \{0, .$ but it is often advantageous to have a symbol for this set rather than sp all its elements. This saves writing and makes specification of algorith implementation of computer code easier.

[11] http://tinyurl.com/nm5587k/wave/wave1D/wave1D_n0.py

The first index in the set will be denoted $\mathcal{I}_x^0$ and the last $\mathcal{I}_x^{-1}$. Sometimes we eed to count from the second element in the set, and the notation $\mathcal{I}_x^+$ is then sed. Correspondingly, $\mathcal{I}_x^-$ means $\{0,\ldots,N_x-1\}$. All the indices corresponding o inner grid points are $\mathcal{I}_x^i = \{1,\ldots,N_x-1\}$. For the time domain we find it atural to explicitly use 0 as the first index, so we will usually write $n=0$ and rather than $n=\mathcal{I}_t^0$. We also avoid notation like $x_{\mathcal{I}_x^{-1}}$ and will instead use x_i, $=\mathcal{I}_x^{-1}$.

The Python code associated with index sets applies the following conventions:

Notation	Python
$\mathcal{I}_x$	`Ix`
$\mathcal{I}_x^0$	`Ix[0]`
$\mathcal{I}_x^{-1}$	`Ix[-1]`
$\mathcal{I}_x^-$	`Ix[:-1]`
$\mathcal{I}_x^+$	`Ix[1:]`
$\mathcal{I}_x^i$	`Ix[1:-1]`

n important feature of the index set notation is that it keeps our formulas and ode independent of how we count mesh points. For example, the notation $i\in\mathcal{I}_x$ r $i=\mathcal{I}_x^0$ remains the same whether $\mathcal{I}_x$ is defined as above or as starting at 1, e., $\mathcal{I}_x=\{1,\ldots,Q\}$. Similarly, we can in the code define `Ix=range(Nx+1)` or `x=range(1,Q)`, and expressions like `Ix[0]` and `Ix[1:-1]` remain correct. One pplication where the index set notation is convenient is conversion of code from language where arrays has base index 0 (e.g., Python and C) to languages here the base index is 1 (e.g., MATLAB and Fortran). Another important pplication is implementation of Neumann conditions via ghost points (see next ection).

For the current problem setting in the x,t plane, we work with the index sets

$$\mathcal{I}_x=\{0,\ldots,N_x\},\quad \mathcal{I}_t=\{0,\ldots,N_t\}, \tag{40}$$

efined in Python as

```
Ix = range(0, Nx+1)
It = range(0, Nt+1)
```

A finite difference scheme can with the index set notation be specified as

$$\begin{aligned}
u_i^{n+1} &= -u_i^{n-1} + 2u_i^n + C^2\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right), \quad i\in\mathcal{I}_x^i,\ n\in\mathcal{I}_t^i,\\
u_i &= 0, \quad i=\mathcal{I}_x^0,\ n\in\mathcal{I}_t^i,\\
u_i &= 0, \quad i=\mathcal{I}_x^{-1},\ n\in\mathcal{I}_t^i,
\end{aligned}$$

nd implemented by code like


```
for n in It[1:-1]:
    for i in Ix[1:-1]:
        u[i] = - u_2[i] + 2*u_1[i] + \
               C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1])
    i = Ix[0];  u[i] = 0
    i = Ix[-1]; u[i] = 0
```

Notice.

The program `wave1D_dn.py`[a] applies the index set notation and solve 1D wave equation $u_{tt}=c^2u_{xx}+f(x,t)$ with quite general boundary initial conditions:

- $x=0$: $u=U_0(t)$ or $u_x=0$
- $x=L$: $u=U_L(t)$ or $u_x=0$
- $t=0$: $u=I(x)$
- $t=0$: $u_t=I(x)$

The program combines Dirichlet and Neumann conditions, scalar vectorized implementation of schemes, and the index notation into piece of code. A lot of test examples are also included in the progra

- A rectangular plug profile as initial condition (easy to use as example as the rectangle should jump one cell per time step $C=1$, without any numerical errors).
- A Gaussian function as initial condition.
- A triangular profile as initial condition, which resembles the ty initial shape of a guitar string.
- A sinusoidal variation of u at $x=0$ and either $u=0$ or $u_x=$ $x=L$.
- An exact analytical solution $u(x,t)=\cos(m\pi t/L)\sin(\frac{1}{2}m\pi$ which can be used for convergence rate tests.

[a] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_dn.py`

6.5 Alternative implementation via ghost cells

Idea. Instead of modifying the scheme at the boundary, we can introdu points outside the domain such that the fictitious values u_{-1}^n and u_N^n

efined in the mesh. Adding the intervals $[-\Delta x, 0]$ and $[L, L+\Delta x]$, often referred
o as *ghost cells*, to the mesh gives us all the needed mesh points, corresponding
o $i = -1, 0, \ldots, N_x, N_x+1$. The extra points $i = -1$ and $i = N_x+1$ are known
s *ghost points*, and values at these points, u^n_{-1} and $u^n_{N_x+1}$, are called *ghost*
alues.

The important idea is to ensure that we always have

$$u^n_{-1} = u^n_1 \text{ and } u^n_{N_x+1} = u^n_{N_x-1},$$

ecause then the application of the standard scheme at a boundary point $i = 0$
r $i = N_x$ will be correct and guarantee that the solution is compatible with the
oundary condition $u_x = 0$.

mplementation. The `u` array now needs extra elements corresponding to
he ghost cells and points. Two new point values are needed:

```
u   = zeros(Nx+3)
```

he arrays `u_1` and `u_2` must be defined accordingly.

Unfortunately, a major indexing problem arises with ghost cells. The reason
that Python indices *must* start at 0 and `u[-1]` will always mean the last
ement in `u`. This fact gives, apparently, a mismatch between the mathematical
ndices $i = -1, 0, \ldots, N_x+1$ and the Python indices running over `u`: `0,..,Nx+2`.
ne remedy is to change the mathematical notation of the scheme, as in

$$u^{n+1}_i = \cdots, \quad i = 1, \ldots, N_x+1,$$

eaning that the ghost points correspond to $i = 0$ and $i = N_x+1$. A better
olution is to use the ideas of Section 6.4: we hide the specific index value in
n index set and operate with inner and boundary points using the index set
otation.

To this end, we define `u` with proper length and `Ix` to be the corresponding
ndices for the real physical points $(1, 2, \ldots, N_x+1)$:

```
u = zeros(Nx+3)
Ix = range(1, u.shape[0]-1)
```

hat is, the boundary points have indices `Ix[0]` and `Ix[-1]` (as before). We
rst update the solution at all physical mesh points (i.e., interior points in the
esh extended with ghost cells):

```
for i in Ix:
    u[i] = - u_2[i] + 2*u_1[i] + \
           C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1])
```

remains to update the ghost points. For a boundary condition $u_x = 0$, the
host value must equal to the value at the associated inner mesh point. Computer
ode makes this statement precise:


```
i = Ix[0]          # x=0 boundary
u[i-1] = u[i+1]
i = Ix[-1]         # x=L boundary
u[i+1] = u[i-1]
```

The physical solution to be plotted is now in `u[1:-1]`, or equi
`u[Ix[0]:Ix[-1]+1]`, so this slice is the quantity to be returned from
function. A complete implementation appears in the program `wave1D_n0`
`py`[12].

Warning.

We have to be careful with how the spatial and temporal mesh point
stored. Say we let `x` be the physical mesh points,

```
x = linspace(0, L, Nx+1)
```

"Standard coding" of the initial condition,

```
for i in Ix:
    u_1[i] = I(x[i])
```

becomes wrong, since `u_1` and `x` have different lengths and the inc
corresponds to two different mesh points. In fact, `x[i]` correspon
`u[1+i]`. A correct implementation is

```
for i in Ix:
    u_1[i] = I(x[i-Ix[0]])
```

Similarly, a source term usually coded as `f(x[i], t[n])` is incorrect i
defined to be the physical points, so `x[i]` must be replaced by `x[i-Ix`

An alternative remedy is to let `x` also cover the ghost points such
`u[i]` is the value at `x[i]`.

The ghost cell is only added to the boundary where we have a N
condition. Suppose we have a Dirichlet condition at $x = L$ and a homo
Neumann condition at $x = 0$. One ghost cell $[-\Delta x, 0]$ is added to th
so the index set for the physical points becomes $\{1, \ldots, N_x+1\}$. A
implementation is

```
u = zeros(Nx+2)
Ix = range(1, u.shape[0])
...
for i in Ix[:-1]:
    u[i] = - u_2[i] + 2*u_1[i] + \
           C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1]) + \
           dt2*f(x[i-Ix[0]], t[n])
```

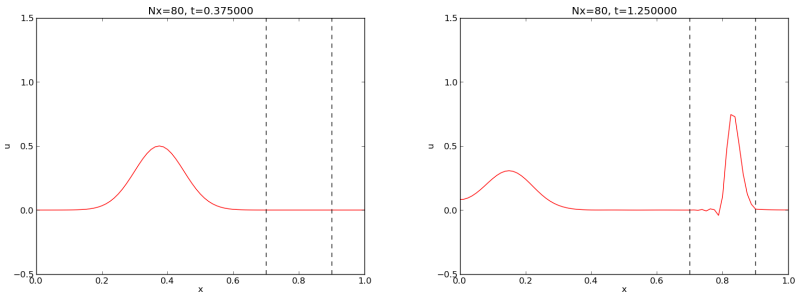
[12] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_n0_ghost.py`

```
i = Ix[-1]
u[i] = U_0       # set Dirichlet value
i = Ix[0]
u[i-1] = u[i+1]  # update ghost value
```

he physical solution to be plotted is now in `u[1:]` or (as always) `u[Ix[0]:Ix[-1]+1]`

Generalization: variable wave velocity

ur next generalization of the 1D wave equation (1) or (17) is to allow for a ariable wave velocity c: $c = c(x)$, usually motivated by wave motion in a domain omposed of different physical media with different properties for propagating aves and hence different wave velocities c. Figure



igure 5: Left: wave entering another medium; right: transmitted and reflected ave .

.1 The model PDE with a variable coefficient

nstead of working with the squared quantity $c^2(x)$ we shall for notational onvenience introduce $q(x) = c^2(x)$. A 1D wave equation with variable wave elocity often takes the form

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(q(x)\frac{\partial u}{\partial x}\right) + f(x,t)\,. \tag{41}$$

his equation sampled at a mesh point (x_i, t_n) reads

$$\frac{\partial^2}{\partial t^2}u(x_i,t_n) = \frac{\partial}{\partial x}\left(q(x_i)\frac{\partial}{\partial x}u(x_i,t_n)\right) + f(x_i,t_n),$$

here the only new term is

$$\frac{\partial}{\partial x}\left(q(x_i)\frac{\partial}{\partial x}u(x_i,t_n)\right) = \left[\frac{\partial}{\partial x}\left(q(x)\frac{\partial u}{\partial x}\right)\right]_i^n .$$

7.2 Discretizing the variable coefficient

The principal idea is to first discretize the outer derivative. Define

$$\phi = q(x)\frac{\partial u}{\partial x},$$

and use a centered derivative around $x = x_i$ for the derivative of ϕ:

$$\left[\frac{\partial \phi}{\partial x}\right]_i^n \approx \frac{\phi_{i+\frac{1}{2}} - \phi_{i-\frac{1}{2}}}{\Delta x} = [D_x\phi]_i^n\,.$$

Then discretize

$$\phi_{i+\frac{1}{2}} = q_{i+\frac{1}{2}}\left[\frac{\partial u}{\partial x}\right]_{i+\frac{1}{2}}^n \approx q_{i+\frac{1}{2}}\frac{u_{i+1}^n - u_i^n}{\Delta x} = [qD_x u]_{i+\frac{1}{2}}^n\,.$$

Similarly,

$$\phi_{i-\frac{1}{2}} = q_{i-\frac{1}{2}}\left[\frac{\partial u}{\partial x}\right]_{i-\frac{1}{2}}^n \approx q_{i-\frac{1}{2}}\frac{u_i^n - u_{i-1}^n}{\Delta x} = [qD_x u]_{i-\frac{1}{2}}^n\,.$$

These intermediate results are now combined to

$$\left[\frac{\partial}{\partial x}\left(q(x)\frac{\partial u}{\partial x}\right)\right]_i^n \approx \frac{1}{\Delta x^2}\left(q_{i+\frac{1}{2}}\left(u_{i+1}^n - u_i^n\right) - q_{i-\frac{1}{2}}\left(u_i^n - u_{i-1}^n\right)\right)\,.$$

With operator notation we can write the discretization as

$$\left[\frac{\partial}{\partial x}\left(q(x)\frac{\partial u}{\partial x}\right)\right]_i^n \approx [D_x q D_x u]_i^n\,.$$

Remark.

Many are tempted to use the chain rule on the term $\frac{\partial}{\partial x}\left(q(x)\frac{\partial u}{\partial x}\right)$, bu is not a good idea when discretizing such a term.

7.3 Computing the coefficient between mesh points

If q is a known function of x, we can easily evaluate $q_{i+\frac{1}{2}}$ simply as $q(x_{i+}$ $x_{i+\frac{1}{2}} = x_i + \frac{1}{2}\Delta x$. However, in many cases c, and hence q, is only kno discrete function, often at the mesh points x_i. Evaluating q between tv points x_i and x_{i+1} can then be done by averaging in three ways:

$$q_{i+\frac{1}{2}} \approx \frac{1}{2}\left(q_i + q_{i+1}\right) = [\overline{q}^x]_i, \qquad \text{(arithmetic mean)}$$

$$q_{i+\frac{1}{2}} \approx 2\left(\frac{1}{q_i} + \frac{1}{q_{i+1}}\right)^{-1}, \qquad \text{(harmonic mean)}$$

$$q_{i+\frac{1}{2}} \approx \left(q_i q_{i+1}\right)^{1/2}, \qquad \text{(geometric mean)}$$

he arithmetic mean in (44) is by far the most commonly used averaging echnique.

With the operator notation from (44) we can specify the discretization of ne complete variable-coefficient wave equation in a compact way:

$$[D_t D_t u = D_x \overline{q}^x D_x u + f]_i^n \,. \tag{47}$$

rom this notation we immediately see what kind of differences that each term is pproximated with. The notation $\overline{q}^x$ also specifies that the variable coefficient is pproximated by an arithmetic mean, the definition being $[\overline{q}^x]_{i+\frac{1}{2}} = (q_i + q_{i+1})/2$. /ith the notation $[D_x q D_x u]_i^n$, we specify that q is evaluated directly, as a nction, between the mesh points: $q(x_{i-\frac{1}{2}})$ and $q(x_{i+\frac{1}{2}})$.

Before any implementation, it remains to solve (47) with respect to u_i^{n+1}:

$$\begin{aligned} u_i^{n+1} = & -u_i^{n-1} + 2u_i^n + \\ & \left(\frac{\Delta x}{\Delta t}\right)^2 \left(\frac{1}{2}(q_i + q_{i+1})(u_{i+1}^n - u_i^n) - \frac{1}{2}(q_i + q_{i-1})(u_i^n - u_{i-1}^n)\right) + \\ & \Delta t^2 f_i^n \,. \end{aligned} \tag{48}$$

.4 How a variable coefficient affects the stability

he stability criterion derived in Section 10.3 reads $\Delta t \leq \Delta x/c$. If $c = c(x)$, ne criterion will depend on the spatial location. We must therefore choose a t that is small enough such that no mesh cell has $\Delta x/c(x) > \Delta t$. That is, we ust use the largest c value in the criterion:

$$\Delta t \leq \beta \frac{\Delta x}{\max_{x\in[0,L]} c(x)} \,. \tag{49}$$

he parameter β is included as a safety factor: in some problems with a gnificantly varying c it turns out that one must choose $\beta < 1$ to have stable olutions ($\beta = 0.9$ may act as an all-round value).

.5 Neumann condition and a variable coefficient

onsider a Neumann condition $\partial u/\partial x = 0$ at $x = L = N_x \Delta x$, discretized as

$$\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0 \quad u_{i+1}^n = u_{i-1}^n,$$

r $i = N_x$. Using the scheme (48) at the end point $i = N_x$ with $u_{i+1}^n = u_{i-1}^n$ esults in

$$\begin{aligned} u_i^{n+1} = & -u_i^{n-1} + 2u_i^n + \\ & \left(\frac{\Delta x}{\Delta t}\right)^2 \left(q_{i+\frac{1}{2}}(u_{i-1}^n - u_i^n) - q_{i-\frac{1}{2}}(u_i^n - u_{i-1}^n)\right) + \\ & \Delta t^2 f_i^n \\ = & -u_i^{n-1} + 2u_i^n + \left(\frac{\Delta x}{\Delta t}\right)^2 (q_{i+\frac{1}{2}} + q_{i-\frac{1}{2}})(u_{i-1}^n - u_i^n) + \Delta t^2 f_i^n \\ \approx & -u_i^{n-1} + 2u_i^n + \left(\frac{\Delta x}{\Delta t}\right)^2 2q_i(u_{i-1}^n - u_i^n) + \Delta t^2 f_i^n \,. \end{aligned}$$

Here we used the approximation

$$\begin{aligned} q_{i+\frac{1}{2}} + q_{i-\frac{1}{2}} &= q_i + \left(\frac{dq}{dx}\right)_i \Delta x + \left(\frac{d^2q}{dx^2}\right)_i \Delta x^2 + \cdots + \\ & \quad q_i - \left(\frac{dq}{dx}\right)_i \Delta x + \left(\frac{d^2q}{dx^2}\right)_i \Delta x^2 + \cdots \\ &= 2q_i + 2\left(\frac{d^2q}{dx^2}\right)_i \Delta x^2 + \mathcal{O}(\Delta x^4) \\ &\approx 2q_i \,. \end{aligned}$$

An alternative derivation may apply the arithmetic mean of q in (48), to the term

$$(q_i + \frac{1}{2}(q_{i+1} + q_{i-1}))(u_{i-1}^n - u_i^n) \,.$$

Since $\frac{1}{2}(q_{i+1} + q_{i-1}) = q_i + \mathcal{O}(\Delta x^2)$, we end up with $2q_i(u_{i-1}^n - u_i^n)$ for as we did above.

A common technique in implementations of $\partial u/\partial x = 0$ boundary co is to assume $dq/dx = 0$ as well. This implies $q_{i+1} = q_{i-1}$ and $q_{i+1/2} = q_i$ $i = N_x$. The implications for the scheme are

$$\begin{aligned} u_i^{n+1} = & -u_i^{n-1} + 2u_i^n + \\ & \left(\frac{\Delta x}{\Delta t}\right)^2 \left(q_{i+\frac{1}{2}}(u_{i-1}^n - u_i^n) - q_{i-\frac{1}{2}}(u_i^n - u_{i-1}^n)\right) + \\ & \Delta t^2 f_i^n \\ = & -u_i^{n-1} + 2u_i^n + \left(\frac{\Delta x}{\Delta t}\right)^2 2q_{i-\frac{1}{2}}(u_{i-1}^n - u_i^n) + \Delta t^2 f_i^n \,. \end{aligned}$$

.6 Implementation of variable coefficients

he implementation of the scheme with a variable wave velocity may assume
iat c is available as an array `c[i]` at the spatial mesh points. The following
op is a straightforward implementation of the scheme (48):

```
or i in range(1, Nx):
    u[i] = - u_2[i] + 2*u_1[i] + \
           C2*(0.5*(q[i] + q[i+1])*(u_1[i+1] - u_1[i])  - \
               0.5*(q[i] + q[i-1])*(u_1[i] - u_1[i-1])) + \
           dt2*f(x[i], t[n])
```

he coefficient `C2` is now defined as `(dt/dx)**2` and *not* as the squared Courant
umber since the wave velocity is variable and appears inside the parenthesis.

With Neumann conditions $u_x = 0$ at the boundary, we need to combine
iis scheme with the discrete version of the boundary condition, as shown in
ection 7.5. Nevertheless, it would be convenient to reuse the formula for the
iterior points and just modify the indices `ip1=i+1` and `im1=i-1` as we did in
ection 6.3. Assuming $dq/dx = 0$ at the boundaries, we can implement the
cheme at the boundary with the following code.

```
i = 0
ip1 = i+1
im1 = ip1
u[i] = - u_2[i] + 2*u_1[i] + \
       C2*(0.5*(q[i] + q[ip1])*(u_1[ip1] - u_1[i])  - \
           0.5*(q[i] + q[im1])*(u_1[i] - u_1[im1])) + \
       dt2*f(x[i], t[n])
```

With ghost cells we can just reuse the formula for the interior points also
t the boundary, provided that the ghost values of both u and q are correctly
pdated to ensure $u_x = 0$ and $q_x = 0$.

A vectorized version of the scheme with a variable coefficient at internal
oints in the mesh becomes

```
u[1:-1] = - u_2[1:-1] + 2*u_1[1:-1] + \
          C2*(0.5*(q[1:-1] + q[2:])*(u_1[2:] - u_1[1:-1]) -
              0.5*(q[1:-1] + q[:-2])*(u_1[1:-1] - u_1[:-2])) + \
          dt2*f(x[1:-1], t[n])
```

.7 A more general model PDE with variable coefficients

ometimes a wave PDE has a variable coefficient also in front of the time-
erivative term:

$$\varrho(x)\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(q(x)\frac{\partial u}{\partial x}\right) + f(x,t)\,. \tag{56}$$

natural scheme is

$$[\varrho D_t D_t u = D_x \overline{q}^x D_x u + f]_i^n\,.$$

We realize that the ϱ coefficient poses no particular difficulty because t
value ϱ_i^n enters the formula above (when written out). There is hence no
any averaging of ϱ. Often, ϱ will be moved to the right-hand side, also
any difficulty:

$$[D_t D_t u = \varrho^{-1} D_x \overline{q}^x D_x u + f]_i^n\,.$$

7.8 Generalization: damping

Waves die out by two mechanisms. In 2D and 3D the energy of the wave
out in space, and energy conservation then requires the amplitude to d
This effect is not present in 1D. Damping is another cause of amplitude re
For example, the vibrations of a string die out because of damping du
resistance and non-elastic effects in the string.

The simplest way of including damping is to add a first-order deriv
the equation (in the same way as friction forces enter a vibrating mec
system):

$$\frac{\partial^2 u}{\partial t^2} + b\frac{\partial u}{\partial t} = c^2\frac{\partial^2 u}{\partial x^2} + f(x,t),$$

where $b \geq 0$ is a prescribed damping coefficient.

A typical discretization of (59) in terms of centered differences read

$$[D_t D_t u + bD_{2t} u = c^2 D_x D_x u + f]_i^n\,.$$

Writing out the equation and solving for the unknown u_i^{n+1} gives the s

$$u_i^{n+1} = (1+\frac{1}{2}b\Delta t)^{-1}((\frac{1}{2}b\Delta t - 1)u_i^{n-1} + 2u_i^n + C^2\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right) +$$

for $i \in \mathcal{I}_x^i$ and $n \geq 1$. New equations must be derived for u_i^1, and for bo
points in case of Neumann conditions.

The damping is very small in many wave phenomena and then only
for very long time simulations. This makes the standard wave equation
damping relevant for a lot of applications.

8 Building a general 1D wave equation sol

The program `wave1D_dn_vc.py`[13] is a fairly general code for 1D wave prop
problems that targets the following initial-boundary value problem

[13] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_dn_vc.py`

$$u_t = (c^2(x)u_x)_x + f(x,t), \qquad x \in (0,L),\ t \in (0,T] \tag{62}$$
$$u(x,0) = I(x), \qquad x \in [0,L] \tag{63}$$
$$u_t(x,0) = V(t), \qquad x \in [0,L] \tag{64}$$
$$u(0,t) = U_0(t) \text{ or } u_x(0,t) = 0, \qquad t \in (0,T] \tag{65}$$
$$u(L,t) = U_L(t) \text{ or } u_x(L,t) = 0, \qquad t \in (0,T] \tag{66}$$

The `solver` function is a natural extension of the simplest `solver` function in ıe initial `wave1D_u0.py` program, extended with Neumann boundary conditions $_x = 0$), a possibly time-varying boundary condition on u ($U_0(t)$, $U_L(t)$), and variable wave velocity. The different code segments needed to make these xtensions are shown and commented upon in the preceding text.

The vectorization is only applied inside the time loop, not for the initial ɔndition or the first time steps, since this initial work is negligible for long time mulations in 1D problems.

The following sections explain various more advanced programming techniques pplied in the general 1D wave equation solver.

.1 User action function as a class

useful feature in the `wave1D_dn_vc.py` program is the specification of the `ser_action` function as a class. Although the `plot_u` function in the `viz` ınction of previous `wave1D*.py` programs remembers the local variables in the `iz` function, it is a cleaner solution to store the needed variables together with ıe function, which is exactly what a class offers.

A class for flexible plotting, cleaning up files, and making a movie files like ınction `viz` and `plot_u` did can be coded as follows:

```
class PlotSolution:
    """
    Class for the user_action function in solver.
    Visualizes the solution only.
    """
    def __init__(self,
                 casename='tmp',    # Prefix in filenames
                 umin=-1, umax=1,   # Fixed range of y axis
                 pause_between_frames=None,  # Movie speed
                 backend='matplotlib',       # or 'gnuplot'
                 screen_movie=True, # Show movie on screen?
                 title='',          # Extra message in title
                 every_frame=1):    # Show every_frame frame
        self.casename = casename
        self.yaxis = [umin, umax]
        self.pause = pause_between_frames
        module = 'scitools.easyviz.' + backend + '_'
        exec('import %s as plt' % module)
        self.plt = plt
        self.screen_movie = screen_movie
        self.title = title
        self.every_frame = every_frame
```



```
        # Clean up old movie frames
        for filename in glob('frame_*.png'):
            os.remove(filename)

    def __call__(self, u, x, t, n):
        if n % self.every_frame != 0:
            return
        title = 't=%.3g' % t[n]
        if self.title:
            title = self.title + ' ' + title
        self.plt.plot(x, u, 'r-',
                      xlabel='x', ylabel='u',
                      axis=[x[0], x[-1],
                            self.yaxis[0], self.yaxis[1]],
                      title=title,
                      show=self.screen_movie)
        # pause
        if t[n] == 0:
            time.sleep(2)  # let initial condition stay 2 s
        else:
            if self.pause is None:
                pause = 0.2 if u.size < 100 else 0
            time.sleep(pause)

        self.plt.savefig('%s_frame_%04d.png' % (self.casename, n))
```

Understanding this class requires quite some familiarity with Python in and class programming in particular.

The constructor shows how we can flexibly import the plotting er (typically) `scitools.easyviz.gnuplot_` or `scitools.easyviz.matpl` (note the trailing underscore). With the `screen_movie` parameter suppress displaying each movie frame on the screen. Alternatively, movies associated with fine meshes, one can set `every_frame` to, e.g., 10, every 10 frames to be shown.

The `__call__` method makes `PlotSolution` instances behave like fu so we can just pass an instance, say `p`, as the `user_action` argumen `solver` function, and any call to `user_action` will be a call to `p.__ca`

8.2 Pulse propagation in two media

The function `pulse` in `wave1D_dn_vc.py` demonstrates wave motion in h neous media where c varies. One can specify an interval where the wave is decreased by a factor `slowness_factor` (or increased by making thi less than one). Four types of initial conditions are available: a rect pulse (`plug`), a Gaussian function (`gaussian`), a "cosine hat" consistin period of the cosine function (`cosinehat`), and half a period of a "cos (`half-cosinehat`). These peak-shaped initial conditions can be place middle (`loc='center'`) or at the left end (`loc='left'`) of the doma `pulse` function is a flexible tool for playing around with various wave and location of a medium with a different wave velocity:

```
def pulse(C=1, Nx=200, animate=True, version='vectorized', T=2,
          loc='center', pulse_tp='gaussian', slowness_factor=2,
          medium=[0.7, 0.9], every_frame=1, sigma=0.05):
    """
    Various peaked-shaped initial conditions on [0,1].
    Wave velocity is decreased by the slowness_factor inside
    medium. The loc parameter can be 'center' or 'left',
    depending on where the initial pulse is to be located.
    The sigma parameter governs the width of the pulse.
    """
    # Use scaled parameters: L=1 for domain length, c_0=1
    # for wave velocity outside the domain.
    L = 1.0
    c_0 = 1.0
    if loc == 'center':
        xc = L/2
    elif loc == 'left':
        xc = 0

    if pulse_tp in ('gaussian','Gaussian'):
        def I(x):
            return exp(-0.5*((x-xc)/sigma)**2)
    elif pulse_tp == 'plug':
        def I(x):
            return 0 if abs(x-xc) > sigma else 1
    elif pulse_tp == 'cosinehat':
        def I(x):
            # One period of a cosine
            w = 2
            a = w*sigma
            return 0.5*(1 + cos(pi*(x-xc)/a)) \
                   if xc - a <= x <= xc + a else 0

    elif pulse_tp == 'half-cosinehat':
        def I(x):
            # Half a period of a cosine
            w = 4
            a = w*sigma
            return cos(pi*(x-xc)/a) \
                   if xc - 0.5*a <= x <= xc + 0.5*a else 0
    else:
        raise ValueError('Wrong pulse_tp="%s"' % pulse_tp)

    def c(x):
        return c_0/slowness_factor \
               if medium[0] <= x <= medium[1] else c_0

    umin=-0.5; umax=1.5*I(xc)
    casename = '%s_Nx%s_sf%s' % \
               (pulse_tp, Nx, slowness_factor)
    action = PlotMediumAndSolution(
        medium, casename=casename, umin=umin, umax=umax,
        every_frame=every_frame, screen_movie=animate)

    dt = (L/Nx)/c  # choose the stability limit with given Nx
    # Lower C will then use this dt, but smaller Nx
    solver(I=I, V=None, f=None, c=c, U_0=None, U_L=None,
           L=L, dt=dt, C=C, T=T,
           user_action=action, version=version,
           stability_safety_factor=1)
```


The `PlotMediumAndSolution` class used here is a subclass of `PlotSc` where the medium with reduced c value, as specified by the `medium` int visualized in the plots.

Notice.

The argument N_x in the `pulse` function does not correspond to the a spatial resolution of $C < 1$, since the `solver` function takes a fixe and C, and adjusts Δx accordingly. As seen in the `pulse` function specified Δt is chosen according to the limit $C = 1$, so if $C < 1$, Δt rer the same, but the `solver` function operates with a larger Δx and sn N_x than was specified in the call to `pulse`. The practical reason is we always want to keep Δt fixed such that plot frames and movie synchronized in time regardless of the value of C (i.e., Δx is varies the Courant number varies).

The reader is encouraged to play around with the `pulse` function:

```
>>> import wave1D_dn_vc as w
>>> w.pulse(loc='left', pulse_tp='cosinehat', Nx=50, every_frame=
```

To easily kill the graphics by Ctrl-C and restart a new simulation it m easier to run the above two statements from the command line with

```
Terminal> python -c 'import wave1D_dn_vc as w; w.pulse(...)'
```

9 Exercises

Exercise 6: Find the analytical solution to a damped equation

Consider the wave equation with damping (59). The goal is to find a solution to a wave problem with damping. A starting point is the standi solution from Exercise 1. It becomes necessary to include a damping te and also have both a sine and cosine component in time:

$$u_{\mathrm{e}}(x,t) = e^{-\beta t}\sin kx\left(A\cos\omega t + B\sin\omega t\right)\ .$$

Find k from the boundary conditions $u(0,t) = u(L,t) = 0$. Then use t to find constraints on β, ω, A, and B. Set up a complete initial-boundai problem and its solution. Filename: `damped_waves.pdf`.

Problem 7: Explore symmetry boundary conditions

Consider the simple "plug" wave where $\Omega = [-L, L]$ and

$$I(x) = \begin{cases} 1, & x \in [-\delta, \delta], \\ 0, & \text{otherwise} \end{cases}$$

for some number $0 < \delta < L$. The other initial condition is $u_t(x, 0) = 0$ and there is no source term f. The boundary conditions can be set to $u = 0$. The solution to this problem is symmetric around $x = 0$. This means that we can simulate the wave process in only the half of the domain $[0, L]$.

a) Argue why the symmetry boundary condition is $u_x = 0$ at $x = 0$.

Hint. Symmetry of a function about $x = x_0$ means that $f(x_0 + h) = f(x_0 - h)$.

b) Perform simulations of the complete wave problem from on $[-L, L]$. Thereafter, utilize the symmetry of the solution and run a simulation in half of the domain $[0, L]$, using a boundary condition at $x = 0$. Compare the two solutions and make sure that they are the same.

c) Prove the symmetry property of the solution by setting up the complete initial-boundary value problem and showing that if $u(x, t)$ is a solution, then also $u(-x, t)$ is a solution.
Filename: `wave1D_symmetric`.

Exercise 8: Send pulse waves through a layered medium

Use the `pulse` function in `wave1D_dn_vc.py` to investigate sending a pulse, located with its peak at $x = 0$, through the medium to the right where it hits another medium for $x \in [0.7, 0.9]$ where the wave velocity is decreased by a factor s_f. Report what happens with a Gaussian pulse, a "cosine hat" pulse, half a "cosine hat" pulse, and a plug pulse for resolutions $N_x = 40, 80, 160$, and $s_f = 2, 4$. Use $C = 1$ in the medium outside $[0.7, 0.9]$. Simulate until $T = 2$.
Filename: `pulse1D.py`.

Exercise 9: Compare discretizations of a Neumann condition

We have a 1D wave equation with variable wave velocity: $u_t = (qu_x)_x$. A Neumann condition u_x at $x = 0, L$ can be discretized as shown in (52) and (55).

The aim of this exercise is to examine the rate of the numerical error when using different ways of discretizing the Neumann condition. As test problem, $q = 1 + (x - L/2)^4$ can be used, with $f(x, t)$ adapted such that the solution has a simple form, say $u(x, t) = \cos(\pi x/L)\cos(\omega t)$ for some $\omega = \sqrt{q}\pi/L$.

a) Perform numerical experiments and find the convergence rate of the error using the approximation and (55).

b) Switch to $q(x) = \cos(\pi x/L)$, which is symmetric at $x = 0, L$, and ch convergence rate of the scheme (55). Now, $q_{i-1/2}$ is a 2nd-order approxim q_i, $q_{i-1/2} = q_i + 0.25q_i''\Delta x^2 + \cdots$, because $q_i' = 0$ for $i = N_x$ (a similar an can be applied to the case $i = 0$).

c) A third discretization can be based on a simple and convenient, accurate, one-sided difference: $u_i - u_{i-1} = 0$ at $i = N_x$ and $u_{i+1} - u_i$ $i = 0$. Derive the resulting scheme in detail and implement it. Run expe to establish the rate of convergence.

d) A fourth technique is to view the scheme as

$$[D_t D_t u]_i^n = \frac{1}{\Delta x}\left([qD_x u]_{i+\frac{1}{2}}^n - [qD_x u]_{i-\frac{1}{2}}^n\right) + [f]_i^n,$$

and place the boundary at $x_{i+\frac{1}{2}}$, $i = N_x$, instead of exactly at the boundary. With this idea, we can just set $[qD_x u]_{i+\frac{1}{2}}^n = 0$. Derive the c scheme using this technique. The implementation of the boundary cond $L - \Delta x/2$ is $\mathcal{O}(\Delta x^2)$ accurate, but the interesting question is what imp movement of the boundary has on the convergence rate (compute the e usual over the entire mesh).

Exercise 10: Verification by a cubic polynomial in sp

The purpose of this exercise is to verify the implementation of the function in the program `wave1D_n0.py`[14] by using an exact numerical for the wave equation $u_{tt} = c^2 u_{xx} + f$ with Neumann boundary co $u_x(0, t) = u_x(L, t) = 0$.

A similar verification is used in the file `wave1D_u0.py`[15], which so same PDE, but with Dirichlet boundary conditions $u(0, t) = u(L, t) =$ idea of the verification test in function `test_quadratic` in `wave1D_u0.` a solution that is a lower-order polynomial such that both the PDE prob boundary conditions, and all the discrete equations are exactly fulfille the `solver` function should reproduce this exact solution to machine p More precisely, we seek $u = X(x)T(t)$, with $T(t)$ as a linear function a as a parabola that fulfills the boundary conditions. Inserting this u in t determines f. It tuns out that u also fulfills the discrete equations, bec truncation error of the discretized PDE has derivatives in x and t of or and higher. These derivatives all vanish for a quadratic $X(x)$ and linea

It would be attractive to use a similar approach in the case of N conditions. We set $u = X(x)T(t)$ and seek lower-order polynomials X To force u_x to vanish at the boundary, we let X_x be a parabola. The cubic polynomial. The fourth-order derivative of a cubic polynomial van $u = X(x)T(t)$ will fulfill the discretized PDE also in this case, if f is a such that u fulfills the PDE.

[14] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_n0.py`
[15] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_u0.py`

However, the discrete boundary condition is not exactly fulfilled by this
ıoice of u. The reason is that

$$[D_{2x}u]_i^n = u_x(x_i,t_n) + \frac{1}{6}u_{xxx}(x_i,t_n)\Delta x^2 + \mathcal{O}(\Delta x^4)\,. \tag{67}$$

t the boundary two boundary points, $X_x(x) = 0$ such that $u_x = 0$. However,
$_{xxx}$ is a constant and not zero when $X(x)$ is a cubic polynomial. Therefore,
ur $u = X(x)T(t)$ fulfills

$$[D_{2x}u]_i^n = \frac{1}{6}u_{xxx}(x_i,t_n)\Delta x^2,$$

nd not

$$[D_{2x}u]_i^n = 0, quadi = 0, N_x,$$

s it should. (Note that all the higher-order terms $\mathcal{O}(\Delta x^4)$ also have higher-
rder derivatives that vanish for a cubic polynomial.) So to summarize, the
ındamental problem is that u as a product of a cubic polynomial and a linear
r quadratic polynomial in time is not an exact solution of the discrete boundary
ɔnditions.

To make progress, we assume that $u = X(x)T(t)$, where T for simplicity is
ıken as a prescribed linear function $1 + \frac{1}{2}t$, and $X(x)$ is taken as an *unknown*
ıbic polynomial $\sum_{j=0}^{3} a_j x^j$. There are two different ways of determining the
ɔefficients $a_0, \ldots, a_3$ such that both the discretized PDE and the discretized
oundary conditions are fulfilled, under the constraint that we can specify a
ınction $f(x,t)$ for the PDE to feed to the `solver` function in `wave1D_n0.py`.
oth approaches are explained in the subexercises.

) One can insert u in the discretized PDE and find the corresponding f. Then
ne can insert u in the discretized boundary conditions. This yields two equations
ɔr the four coefficients $a_0, \ldots, a_3$. To find the coefficients, one can set $a_0 = 0$
nd $a_1 = 1$ for simplicity and then determine a_2 and a_3. This approach will
ıake a_2 and a_3 depend on Δx and f will depend on both Δx and Δt.

Use `sympy` to perform analytical computations. A starting point is to define
as follows:

```
ıef test_cubic1():
    import sympy as sm
    x, t, c, L, dx, dt = sm.symbols('x t c L dx dt')
    i, n = sm.symbols('i n', integer=True)

    # Assume discrete solution is a polynomial of degree 3 in x
    T = lambda t: 1 + sm.Rational(1,2)*t  # Temporal term
    a = sm.symbols('a_0 a_1 a_2 a_3')
    X = lambda x: sum(a[q]*x**q for q in range(4))  # Spatial term
    u = lambda x, t: X(x)*T(t)
```

he symbolic expression for u is reached by calling `u(x,t)` with `x` and `t` as
ympy symbols.

Define `DxDx(u, i, n)`, `DtDt(u, i, n)`, and `D2x(u, i, n)` as Pyth
tions for returning the difference approximations $[D_xD_xu]_i^n$, $[D_tD_tu$
$[D_{2x}u]_i^n$. The next step is to set up the residuals for the equations $[D_{2x}$
and $[D_{2x}u]_{N_x}^n = 0$, where $N_x = L/\Delta x$. Call the residuals `R_0` and `R_L`.
tute a_0 and a_1 by 0 and 1, respectively, in `R_0`, `R_L`, and `a`:

```
R_0 = R_0.subs(a[0], 0).subs(a[1], 1)
R_L = R_L.subs(a[0], 0).subs(a[1], 1)
a = list(a)  # enable in-place assignment
a[0:2] = 0, 1
```

Determining a_2 and a_3 from the discretized boundary conditions is the
solving two equations with respect to a_2 and a_3, i.e., `a[2:]`:

```
s = sm.solve([R_0, R_L], a[2:])
# s is dictionary with the unknowns a[2] and a[3] as keys
a[2:] = s[a[2]], s[a[3]]
```

Now, `a` contains computed values and `u` will automatically use these nev
since `X` accesses `a`.

Compute the source term f from the discretized PDE: $f_i^n = [L$
$c^2D_xD_xu]_i^n$. Turn u, the time derivative u_t (needed for the initial conditio
and f into Python functions. Set numerical values for L, N_x, C, and c. P
the time interval as $\Delta t = CL/(N_xc)$, which imply $\Delta x = c\Delta t/C = L/N_x$
new functions `I(x)`, `V(x)`, and `f(x,t)` as wrappers of the ones mad
where fixed values of L, c, Δx, and Δt are inserted, such that `I`, `V`, an
be passed on to the `solver` function. Finally, call `solver` with a `user_`
function that compares the numerical solution to this exact solution
discrete PDE problem.

Hint. To turn a `sympy` expression `e`, depending on a series of symbol
`t`, `dx`, `dt`, `L`, and `c`, into plain Python function `e_exact(x,t,L,dx,dt,`
can write

```
e_exact = sm.lambdify([x,t,L,dx,dt,c], e, 'numpy')
```

The `'numpy'` argument is a good habit as the `e_exact` function will th
with array arguments if it contains mathematical functions (but here we
plain arithmetics, which automatically work with arrays).

b) An alternative way of determining $a_0, \ldots, a_3$ is to reason as follows.
construct $X(x)$ such that the boundary conditions are fulfilled: $X = x$
However, to compensate for the fact that this choice of X does not fu
discrete boundary condition, we seek u such that

$$u_x = \frac{\partial}{\partial x}x(L-x)T(t) - \frac{1}{6}u_{xxx}\Delta x^2,$$

nce this u will fit the discrete boundary condition. Assuming $u = T(t)\sum_{j=0}^{3} a_j x^j$, e can use the above equation to determine the coefficients a_1, a_2, a_3. A value, g., 1 can be used for a_0. The following `sumpy` code computes this u:

```
lef test_cubic2():
    import sympy as sm
    x, t, c, L, dx = sm.symbols('x t c L dx')
    T = lambda t: 1 + sm.Rational(1,2)*t  # Temporal term
    # Set u as a 3rd-degree polynomial in space
    X = lambda x: sum(a[i]*x**i for i in range(4))
    a = sm.symbols('a_0 a_1 a_2 a_3')
    u = lambda x, t: X(x)*T(t)
    # Force discrete boundary condition to be zero by adding
    # a correction term the analytical suggestion x*(L-x)*T
    # u_x = x*(L-x)*T(t) - 1/6*u_xxx*dx**2
    R = sm.diff(u(x,t), x) - (
        x*(L-x) - sm.Rational(1,6)*sm.diff(u(x,t), x, x, x)*dx**2)
    # R is a polynomial: force all coefficients to vanish.
    # Turn R to Poly to extract coefficients:
    R = sm.poly(R, x)
    coeff = R.all_coeffs()
    s = sm.solve(coeff, a[1:])  # a[0] is not present in R
    # s is dictionary with a[i] as keys
    # Fix a[0] as 1
    s[a[0]] = 1
    X = lambda x: sm.simplify(sum(s[a[i]]*x**i for i in range(4)))
    u = lambda x, t: X(x)*T(t)
    print 'u:', u(x,t)
```

The next step is to find the source term `f_e` by inserting `u_e` in the PDE. hereafter, turn `u`, `f`, and the time derivative of `u` into plain Python functions s in a), and then wrap these functions in new functions `I`, `V`, and `f`, with the ght signature as required by the `solver` function. Set parameters as in a) and ıeck that the solution is exact to machine precision at each time level using an ppropriate `user_action` function.
ilename: `wave1D_n0_test_cubic.py`.

.0 Analysis of the difference equations

0.1 Properties of the solution of the wave equation

he wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

as solutions of the form

$$u(x,t) = g_R(x - ct) + g_L(x + ct), \tag{68}$$

ɔr any functions g_R and g_L sufficiently smooth to be differentiated twice. The ɔsult follows from inserting (68) in the wave equation. A function of the form $_R(x - ct)$ represents a signal moving to the right in time with constant velocity

c. This feature can be explained as follows. At time $t = 0$ the signal lo $g_R(x)$. Introducing a moving x axis with coordinates $\xi = x - ct$, we function $g_R(\xi)$ is "at rest" in the ξ coordinate system, and the shape is alv same. Say the $g_R(\xi)$ function has a peak at $\xi = 0$. This peak is located a which means that it moves with the velocity $dx/dt = c$ in the x coo system. Similarly, $g_L(x + ct)$ is a function initially with shape $g_L(x)$ tha in the negative x direction with constant velocity c (introduce $\xi = x +$ at the point $\xi = 0$, $x = -ct$, which has velocity $dx/dt = -c$).

With the particular initial conditions

$$u(x,0) = I(x), \quad \frac{\partial}{\partial t}u(x,0) = 0,$$

we get, with u as in (68),

$$g_R(x) + g_L(x) = I(x), \quad -cg_R'(x) + cg_L'(x) = 0,$$

which have the solution $g_R = g_L = I/2$, and consequently

$$u(x,t) = \frac{1}{2}I(x - ct) + \frac{1}{2}I(x + ct)\,.$$

The interpretation of (69) is that the initial shape of u is split into tw each with the same shape as I but half of the initial amplitude. One traveling to the left and the other one to the right.

The solution has two important physical features: constant amplitud left and right wave, and constant velocity of these two waves. It turns (the numerical solution will also preserve the constant amplitude, but the depends on the mesh parameters Δt and Δx.

The solution (69) will be influenced by boundary conditions when tl $\frac{1}{2}I(x - ct)$ and $\frac{1}{2}I(x + ct)$ hit the boundaries and get, e.g., reflected bɛ the domain. However, when $I(x)$ is nonzero only in a small part in the m the spatial domain $[0, L]$, which means that the boundaries are placed f from the initial disturbance of u, the solution (69) is very clearly obser simulation.

A useful representation of solutions of wave equations is a linear coml of sine and/or cosine waves. Such a sum of waves is a solution if the gc PDE is linear and each sine or cosine wave fulfills the equation. To ease ar calculations by hand we shall work with complex exponential functions of real-valued sine or cosine functions. The real part of complex exp will typically be taken as the physical relevant quantity (whenever a p relevant quantity is strictly needed). The idea now is to build $I(x)$ of (wave components e^{ikx}:

$$I(x) \approx \sum_{k \in K} b_k e^{ikx}\,.$$

Here, k is the frequency of a component, K is some set of all the discrete needed to approximate $I(x)$ well, and b_k are constants that must be det We will very seldom need to compute the b_k coefficients: most of the ins

ook for and the understanding of the numerical methods we want to establish, ome from investigating how the PDE and the scheme treat a single component ^{ikx} wave.

Letting the number of k values in K tend to infinity makes the sum (70) onverge to $I(x)$, and this sum is known as a *Fourier series* representation of (x). Looking at (69), we see that the solution $u(x,t)$, when $I(x)$ is represented s in (70), is also built of basic complex exponential wave components of the orm $e^{ik(x\pm ct)}$ according to

$$u(x,t) = \frac{1}{2}\sum_{k\in K} b_k e^{ik(x-ct)} + \frac{1}{2}\sum_{k\in K} b_k e^{ik(x+ct)}\,. \tag{71}$$

is common to introduce the frequency in time $\omega = kc$ and assume that $u(x,t)$ a sum of basic wave components written as $e^{ikx-\omega t}$. (Observe that inserting uch a wave component in the governing PDE reveals that $\omega^2 = k^2c^2$, or $\omega \pm kc$, eflecting the two solutions: one $(+kc)$ traveling to the right and the other $(-kc)$ raveling to the left.)

0.2 More precise definition of Fourier representations

he quick intuitive introduction above to representing a function by a sum of ne and cosine waves suffices as background for the forthcoming material on nalyzing a single wave component. However, to understand all details of how ifferent wave components sum up to the analytical and numerical solution, a ore precise mathematical treatment is helpful and therefore summarized below.

It is well known that periodic functions can be represented by Fourier series. generalization of the Fourier series idea to non-periodic functions defined on ne real line is the *Fourier transform*:

$$I(x) = \int_{-\infty}^{\infty} A(k)e^{ikx}dk, \tag{72}$$

$$A(k) = \int_{-\infty}^{\infty} I(x)e^{-ikx}dx\,. \tag{73}$$

he function $A(k)$ reflects the weight of each wave component e^{ikx} in an infinite um of such wave components. That is, $A(k)$ reflects the frequency content in ne function $I(x)$. Fourier transforms are particularly fundamental for analyzing nd understanding time-varying signals.

The solution of the linear 1D wave PDE can be expressed as

$$u(x,t) = \int_{-\infty}^{\infty} A(k)e^{i(kx-\omega(k)t)}dx\,.$$

In a finite difference method, we represent u by a mesh function u_q^n, where n ounts temporal mesh points and q counts the spatial ones (the usual counter or spatial points, i, is here already used as imaginary unit). Similarly, $I(x)$

is approximated by the mesh function I_q, $q = 0,\ldots,N_x$. On a mesh, not make sense to work with wave components e^{ikx} for very large k, the shortest possible sine or cosine wave that can be represented on with spacing Δx is the wave with wavelength $2\Delta x$ (the sine/cosin jumps up and down between each mesh point). The corresponding k $k = 2\pi/(2\Delta x) = \pi/\Delta x$, known as the *Nyquist frequency*. Within the r relevant frequencies $(0, \pi/\Delta x]$ one defines the discrete Fourier transform[1] $N_x + 1$ discrete frequencies:

$$I_q = \frac{1}{N_x+1}\sum_{k=0}^{N_x} A_k e^{i2\pi kj/(N_x+1)}, \quad i = 0,\ldots,N_x,$$

$$A_k = \sum_{q=0}^{N_x} I_q e^{-i2\pi kq/(N_x+1)}, \quad k = 0,\ldots,N_x+1\,.$$

The A_k values is the discrete Fourier transform of the I_q values, and th are the inverse discrete Fourier transform of the A_k values.

The discrete Fourier transform is efficiently computed by the *Fast transform* algorithm. For a real function $I(x)$ the relevant Python c computing and plotting the discrete Fourier transform appears in the e below.

```
import numpy as np
from numpy import sin

def I(x):
    return sin(2*pi*x) + 0.5*sin(4*pi*x) + 0.1*sin(6*pi*x)

# Mesh
L = 10; Nx = 100
x = np.linspace(0, L, Nx+1)
dx = L/float(Nx)

# Discrete Fourier transform
A = np.fft.rfft(I(x))
A_amplitude = np.abs(A)

# Compute the corresponding frequencies
freqs = np.linspace(0, pi/dx, A_amplitude.size)

import matplotlib.pyplot as plt
plt.plot(freqs, A_amplitude)
plt.show()
```

10.3 Stability

The scheme

[16] http://en.wikipedia.org/wiki/Discrete_Fourier_transform

$$[D_tD_tu = c^2D_xD_xu]^n_q \tag{76}$$

›r the wave equation $u_t = c^2u_{xx}$ allows basic wave components

$$u^n_q = e^{i(kx_q - \tilde{\omega}t_n)}$$

s solution, but it turns out that the frequency in time, $\tilde{\omega}$, is not equal to the xact $\omega = kc$. The idea now is to study how the scheme treats an arbitrary wave ɔmponent with a given k. We ask two key questions:

- How accurate is $\tilde{\omega}$ compared to ω?
- Does the amplitude of such a wave component preserve its (unit) amplitude, as it should, or does it get amplified or damped in time (due to a complex $\tilde{\omega}$)?

he following analysis will answer these questions. Note the need for using q as ɔunter for the mesh point in x direction since i is already used as the imaginary nit (in this analysis).

'reliminary results. A key result needed in the investigations is the finite ifference approximation of a second-order derivative acting on a complex wave ɔmponent:

$$[D_tD_te^{i\omega t}]^n = -\frac{4}{\Delta t^2}\sin^2\left(\frac{\omega\Delta t}{2}\right)e^{i\omega n\Delta t}\,.$$

y just changing symbols ($\omega \to k$, $t \to x$, $n \to q$) it follows that

$$[D_xD_xe^{ikx}]_q = -\frac{4}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right)e^{ikq\Delta x}\,.$$

Numerical wave propagation. Inserting a basic wave component $u^n_q = e^{i(kx_q - \tilde{\omega}t_n)}$ in (76) results in the need to evaluate two expressions:

$$\begin{aligned}
[D_tD_te^{ikx}e^{-i\tilde{\omega}t}]^n_q &= [D_tD_te^{-i\tilde{\omega}t}]^n e^{ikq\Delta x}\\
&= -\frac{4}{\Delta t^2}\sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right)e^{-i\tilde{\omega}n\Delta t}e^{ikq\Delta x} \qquad (77)\\
[D_xD_xe^{ikx}e^{-i\tilde{\omega}t}]^n_q &= [D_xD_xe^{ikx}]_q e^{-i\tilde{\omega}n\Delta t}\\
&= -\frac{4}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right)e^{ikq\Delta x}e^{-i\tilde{\omega}n\Delta t}\,. \qquad (78)
\end{aligned}$$

hen the complete scheme,

$$[D_tD_te^{ikx}e^{-i\tilde{\omega}t} = c^2D_xD_xe^{ikx}e^{-i\tilde{\omega}t}]^n_q$$

leads to the following equation for the unknown numerical frequency $\tilde{\omega}$ dividing by $-e^{ikx}e^{-i\tilde{\omega}t}$):

$$\frac{4}{\Delta t^2}\sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right) = c^2\frac{4}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right),$$

or

$$\sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right) = C^2\sin^2\left(\frac{k\Delta x}{2}\right),$$

where

$$C = \frac{c\Delta t}{\Delta x}$$

is the Courant number. Taking the square root of (79) yields

$$\sin\left(\frac{\tilde{\omega}\Delta t}{2}\right) = C\sin\left(\frac{k\Delta x}{2}\right),$$

Since the exact ω is real it is reasonable to look for a real solution $\tilde{\omega}$ The right-hand side of (81) must then be in $[-1,1]$ because the sine f on the left-hand side has values in $[-1,1]$ for real $\tilde{\omega}$. The sine functior right-hand side can attain the value 1 when

$$\frac{k\Delta x}{2} = m\frac{\pi}{2}, \quad m \in \mathbb{Z}\,.$$

With $m = 1$ we have $k\Delta x = \pi$, which means that the wavelength λ becomes $2\Delta x$. This is the absolutely shortest wavelength that can be repr on the mesh: the wave jumps up and down between each mesh point. values of $|m|$ are irrelevant since these correspond to k values whose wa too short to be represented on a mesh with spacing Δx. For the shortest wave in the mesh, $\sin(k\Delta x/2) = 1$, and we must require

$$C \leq 1\,.$$

Consider a right-hand side in (81) of magnitude larger than unit solution $\tilde{\omega}$ of (81) must then be a complex number $\tilde{\omega} = \tilde{\omega}_r + i\tilde{\omega}_i$ beca sine function is larger than unity for a complex argument. One can sh for any ω_i there will also be a corresponding solution with $-\omega_i$. The cor with $\omega_i > 0$ gives an amplification factor $e^{\omega_i t}$ that grows exponentially We cannot allow this and must therefore require $C \leq 1$ as a *stability cr*

Remark.

For smoother wave components with longer wave lengths per length (82) can in theory be relaxed. However, small round-off errors are al present in a numerical solution and these vary arbitrarily from mesh to mesh point and can be viewed as unavoidable noise with wavele

$2\Delta x$. As explained, $C > 1$ will for this very small noise lead to exponential growth of the shortest possible wave component in the mesh. This noise will therefore grow with time and destroy the whole solution.

0.4 Numerical dispersion relation

quation (81) can be solved with respect to $\tilde{\omega}$:

$$\tilde{\omega} = \frac{2}{\Delta t}\sin^{-1}\left(C\sin\left(\frac{k\Delta x}{2}\right)\right). \tag{83}$$

he relation between the numerical frequency $\tilde{\omega}$ and the other parameters k, c, x, and Δt is called a *numerical dispersion relation*. Correspondingly, $\omega = kc$ is ıe *analytical dispersion relation*.

The special case $C = 1$ deserves attention since then the right-hand side of 3) reduces to

$$\frac{2}{\Delta t}\frac{k\Delta x}{2} = \frac{1}{\Delta t}\frac{\omega\Delta x}{c} = \frac{\omega}{C} = \omega\,.$$

hat is, $\tilde{\omega} = \omega$ and the numerical solution is exact at all mesh points regardless of x and Δt! This implies that the numerical solution method is also an analytical olution method, at least for computing u at discrete points (the numerical ıethod says nothing about the variation of u *between* the mesh points, and nploying the common linear interpolation for extending the discrete solution ives a curve that deviates from the exact one).

For a closer examination of the error in the numerical dispersion relation hen $C < 1$, we can study $\tilde{\omega} - \omega$, $\tilde{\omega}/\omega$, or the similar error measures in wave elocity: $\tilde{c} - c$ and $\tilde{c}/c$, where $c = \omega/k$ and $\tilde{c} = \tilde{\omega}/k$. It appears that the most onvenient expression to work with is $\tilde{c}/c$:

$$\frac{\tilde{c}}{c} = \frac{1}{Cp}\sin^{-1}\left(C\sin p\right),$$

ith $p = k\Delta x/2$ as a non-dimensional measure of the spatial frequency. In ssence, p tells how many spatial mesh points we have per wave length in space f the wave component with frequency k (the wave length is $2\pi/k$). That is, p eflects how well the spatial variation of the wave component is resolved in the ıesh. Wave components with wave length less than $2\Delta x$ ($2\pi/k < 2\Delta x$) are not isible in the mesh, so it does not make sense to have $p > \pi/2$.

We may introduce the function $r(C,p) = \tilde{c}/c$ for further investigation of umerical errors in the wave velocity:

$$r(C,p) = \frac{1}{Cp}\sin^{-1}\left(C\sin p\right), \quad C \in (0,1],\ p \in (0,\pi/2]\,. \tag{84}$$

his function is very well suited for plotting since it combines several parameters ı the problem into a dependence on two non-dimensional numbers, C and p.

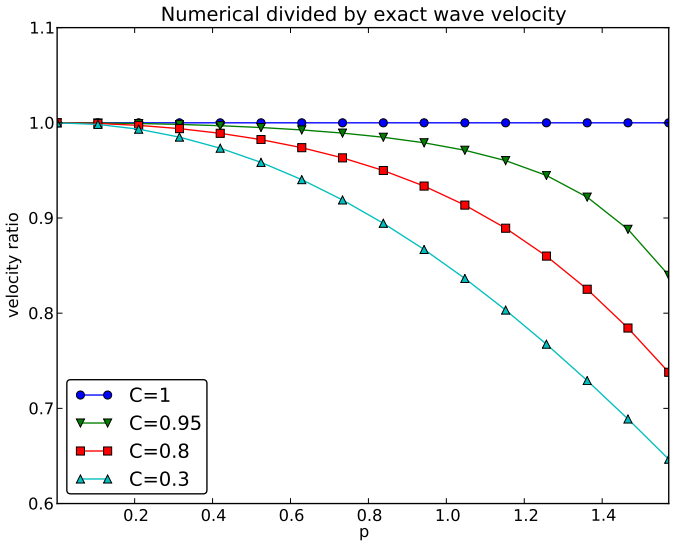


Figure 6: The fractional error in the wave velocity for different Courant r

Defining

```
def r(C, p):
    return 2/(C*p)*asin(C*sin(p))
```

we can plot $r(C,p)$ as a function of p for various values of C, see Figure that the shortest waves have the most erroneous velocity, and that shoı move more slowly than they should.

With `sympy` we can also easily make a Taylor series expansion in cretization parameter p:

```
>>> C, p = symbols('C p')
>>> # Compute the 7 first terms around p=0 with no O() term
>>> rs = r(C, p).series(p, 0, 7).removeO()
>>> rs
p**6*(5*C**6/112 - C**4/16 + 13*C**2/720 - 1/5040) +
p**4*(3*C**4/40 - C**2/12 + 1/120) +
p**2*(C**2/6 - 1/6) + 1
>>> rs_error_leading_order = (rs - 1).extract_leading_order(p)
>>> rs_error_leading_order
p**2*(C**2/6 - 1/6)
>>> # Turn the series expansion into a Python function
>>> rs_pyfunc = lambdify([C, p], rs, modules='numpy')
>>> # Check: rs_pyfunc is exact (=1) for C=1
>>> rs_pyfunc(1, 0.1)
1.0
```

Without the `.removeO()` call the series get an `O(x**7)` term that makes it impossible to convert the series to a Python function (for, e.g., plotting).

From the `rs_error_leading_order` expression above we see that the leading order term in the error of this series expansion is

$$\frac{1}{6}\left(\frac{k\Delta x}{2}\right)^2 (C^2-1) = \frac{k^2}{24}\left(c^2\Delta t^2 - \Delta x^2\right), \tag{85}$$

pointing to an error $\mathcal{O}(\Delta t^2, \Delta x^2)$, which is compatible with the errors in the difference approximations (D_tD_t and D_xD_x).

Here is an alternative way of performing a series expansion: we use the `series` method, which returns an iterator over all the terms in the expansion, and ask for the 4 first terms (via `itertools.islice`, which can slice an iterator). Collecting the terms in a list makes it possible to factor each term individually. Summing up the terms results in a nicer expression:

```
>>> import itertools
>>> rs = [t for t in itertools.islice(r(C, p).lseries(p), 4)]
>>> rs
[1, C**2*p**2/6 - p**2/6,
 3*C**4*p**4/40 - C**2*p**4/12 + p**4/120,
 5*C**6*p**6/112 - C**4*p**6/16 + 13*C**2*p**6/720 - p**6/5040]
>>> rs = [factor(t) for t in rs]
>>> rs
[1, p**2*(C - 1)*(C + 1)/6,
 p**4*(C - 1)*(C + 1)*(3*C - 1)*(3*C + 1)/120,
 p**6*(C - 1)*(C + 1)*(225*C**4 - 90*C**2 + 1)/5040]
>>> rs = sum(rs)  # Python's sum function
>>> rs
p**6*(C - 1)*(C + 1)*(225*C**4 - 90*C**2 + 1)/5040 +
p**4*(C - 1)*(C + 1)*(3*C - 1)*(3*C + 1)/120 +
p**2*(C - 1)*(C + 1)/6 + 1
```

We see from the last expression that $C = 1$ makes all the terms in `rs` vanish. Since we already know that the numerical solution is exact for $C = 1$, the remaining terms in the Taylor series expansion will also contain factors of $C - 1$ and cancel for $C = 1$.

0.5 Extending the analysis to 2D and 3D

The typical analytical solution of a 2D wave equation

$$u_{tt} = c^2(u_{xx} + u_{yy}),$$

is a wave traveling in the direction of $\boldsymbol{k} = k_x\boldsymbol{i} + k_y\boldsymbol{j}$, where $\boldsymbol{i}$ and $\boldsymbol{j}$ are unit vectors in the x and y directions, respectively. Such a wave can be expressed by

$$u(x, y, t) = g(k_x x + k_y y - kct)$$

for some twice differentiable function g, or with $\omega = kc$, $k = |\boldsymbol{k}|$:

$$u(x, y, t) = g(k_x x + k_y y - \omega t)\,.$$

We can in particular build a solution by adding complex Fourier compo the form

$$\exp\left(i(k_x x + k_y y - \omega t)\right).$$

A discrete 2D wave equation can be written as

$$[D_tD_t u = c^2(D_xD_x u + D_yD_y u)]^n_{q,r}\,.$$

This equation admits a Fourier component

$$u^n_{q,r} = \exp\left(i(k_x q\Delta x + k_y r\Delta y - \tilde{\omega} n\Delta t)\right),$$

as solution. Letting the operators D_tD_t, D_xD_x, and D_yD_y act on $u^n_{q,r}$ fi transforms (86) to

$$\frac{4}{\Delta t^2}\sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right) = c^2\frac{4}{\Delta x^2}\sin^2\left(\frac{k_x\Delta x}{2}\right) + c^2\frac{4}{\Delta y^2}\sin^2\left(\frac{k_y\Delta y}{2}\right).$$

or

$$\sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right) = C_x^2\sin^2 p_x + C_y^2\sin^2 p_y,$$

where we have eliminated the factor 4 and introduced the symbols

$$C_x = \frac{c^2\Delta t^2}{\Delta x^2}, \quad C_y = \frac{c^2\Delta t^2}{\Delta y^2}, \quad p_x = \frac{k_x\Delta x}{2}, \quad p_y = \frac{k_y\Delta y}{2}.$$

For a real-valued $\tilde{\omega}$ the right-hand side must be less than or equal to absolute value, requiring in general that

$$C_x^2 + C_y^2 \leq 1\,.$$

This gives the stability criterion, more commonly expressed directl inequality for the time step:

$$\Delta t \leq \frac{1}{c}\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)^{-1/2}$$

A similar, straightforward analysis for the 3D case leads to

$$\Delta t \leq \frac{1}{c}\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}\right)^{-1/2}$$

In the case of a variable coefficient $c^2 = c^2(\boldsymbol{x})$, we must use the worst-ca

$$\bar{c} = \sqrt{\max_{\boldsymbol{x}\in\Omega} c^2(\boldsymbol{x})}$$

in the stability criteria. Often, especially in the variable wave velocity ca wise to introduce a safety factor $\beta \in (0, 1]$ too:

$$\Delta t \leq \beta \frac{1}{\tilde{c}} \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)^{-1/2} \tag{94}$$

The exact numerical dispersion relations in 2D and 3D becomes, for constant

$$\tilde{\omega} = \frac{2}{\Delta t} \sin^{-1} \left(\left(C_x^2 \sin^2 p_x + C_y^2 \sin_y^p \right)^{\frac{1}{2}} \right), \tag{95}$$

$$\tilde{\omega} = \frac{2}{\Delta t} \sin^{-1} \left(\left(C_x^2 \sin^2 p_x + C_y^2 \sin_y^p + C_z^2 \sin_z^p \right)^{\frac{1}{2}} \right). \tag{96}$$

We can visualize the numerical dispersion error in 2D much like we did in 1D. o this end, we need to reduce the number of parameters in $\tilde{\omega}$. The direction of ıe wave is parameterized by the polar angle θ, which means that

$$k_x = k \sin\theta, \quad k_y = k \cos\theta \,.$$

simplification is to set $\Delta x = \Delta y = h$. Then $C_x = C_y = c\Delta t/h$, which we call '. Also,

$$p_x = \frac{1}{2} kh \cos\theta, \quad p_y = \frac{1}{2} kh \sin\theta \,.$$

he numerical frequency $\tilde{\omega}$ is now a function of three parameters:

- C reflecting the number cells a wave is displaced during a time step
- kh reflecting the number of cells per wave length in space
- θ expressing the direction of the wave

/e want to visualize the error in the numerical frequency. To avoid having Δt s a free parameter in $\tilde{\omega}$, we work with $\tilde{c}/c$, because the fraction $2/\Delta t$ is then ewritten as

$$\frac{2}{kc\Delta t} = \frac{2}{2kc\Delta t h/h} = \frac{1}{Ckh},$$

nd

$$\frac{\tilde{c}}{c} = \frac{1}{Ckh} \sin^{-1} \left(C \left(\sin^2(\frac{1}{2} kh \cos\theta) + \sin^2(\frac{1}{2} kh \sin\theta) \right)^{\frac{1}{2}} \right).$$

/e want to visualize this quantity as a function of kh and θ for some values of ' ≤ 1. It is instructive to make color contour plots of $1 - \tilde{c}/c$ in *polar coordinates* ith θ as the angular coordinate and kh as the radial coordinate.

The stability criterion (90) becomes $C \leq C_{\max} = 1/\sqrt{2}$ in the present 2D ase with the C defined above. Let us plot $1 - \tilde{c}/c$ in polar coordinates for ' $_{\max}, 0.9C_{\max}, 0.5C_{\max}, 0.2C_{\max}$. The program below does the somewhat tricky

work in Matplotlib, and the result appears in Figure 7. From the fi clearly see that the maximum C value gives the best results, and tha whose propagation direction makes an angle of 45 degrees with an axis most accurate.

```
def dispersion_relation_2D(kh, theta, C):
    arg = C*sqrt(sin(0.5*kh*cos(theta))**2 +
                 sin(0.5*kh*sin(theta))**2)
    c_frac = 2./(C*kh)*arcsin(arg)

    return c_frac

from numpy import exp, sin, cos, linspace, \
     pi, meshgrid, arcsin, sqrt
r = kh = linspace(0.001, pi, 101)
theta = linspace(0, 2*pi, 51)
r, theta = meshgrid(r, theta)

# Make 2x2 filled contour plots for 4 values of C
import matplotlib.pyplot as plt
C_max = 1/sqrt(2)
C = [[C_max, 0.9*C_max], [0.5*C_max, 0.2*C_max]]
fix, axes = plt.subplots(2, 2, subplot_kw=dict(polar=True))
for row in range(2):
    for column in range(2):
        error = 1 - dispersion_relation_2D(
            kh, theta, C[row][column])
        print error.min(), error.max()
        cax = axes[row][column].contourf(
            theta, r, error, 50, vmin=0, vmax=0.36)
        axes[row][column].set_xticks([])
        axes[row][column].set_yticks([])

# Add colorbar to the last plot
cbar = plt.colorbar(cax)
cbar.ax.set_ylabel('error in wave velocity')
plt.savefig('disprel2D.png')
plt.savefig('disprel2D.pdf')
plt.show()
```

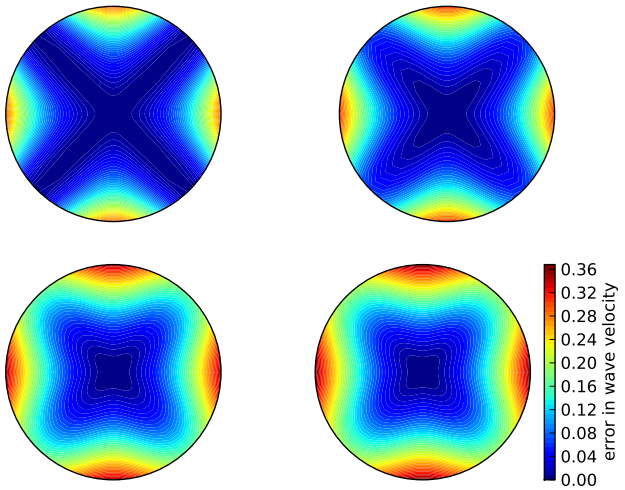


Figure 7: Error in numerical dispersion in 2D.

.1 Finite difference methods for 2D and 3D wave equations

. natural next step is to consider extensions of the methods for various variants of the one-dimensional wave equation to two-dimensional (2D) and three-imensional (3D) versions of the wave equation.

1.1 Multi-dimensional wave equations

he general wave equation in d space dimensions, with constant wave velocity c, an be written in the compact form

$$\frac{\partial^2 u}{\partial t^2} = c^2\nabla^2 u \text{ for } \boldsymbol{x} \in \Omega \subset \mathbb{R}^d,\ t \in (0,T]\,. \tag{97}$$

ı a 2D problem ($d = 2$),

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2},$$

hile in three space dimensions ($d = 3$),

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\,.$$

Many applications involve variable coefficients, and the general wave e in d dimensions is in this case written as

$$\varrho\frac{\partial^2 u}{\partial t^2} = \nabla\cdot(q\nabla u) + f \text{ for } \boldsymbol{x} \in \Omega \subset \mathbb{R}^d,\ t \in (0,T],$$

which in 2D becomes

$$\varrho(x,y)\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(q(x,y)\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(q(x,y)\frac{\partial u}{\partial y}\right) + f(x,y,t)\,.$$

To save some writing and space we may use the index notation, where s t, x, y, or z means differentiation with respect to that coordinate. For e

$$\frac{\partial^2 u}{\partial t^2} = u_{tt},$$
$$\frac{\partial}{\partial y}\left(q(x,y)\frac{\partial u}{\partial y}\right) = (qu_y)_y\,.$$

The 3D versions of the two model PDEs, with and without variable coe can with now with the aid of the index notation for differentiation be s

$$u_{tt} = c^2(u_{xx} + u_{yy} + u_{zz}) + f,$$
$$\varrho u_{tt} = (qu_x)_x + (qu_z)_z + (qu_z)_z + f\,.$$

At *each point* of the boundary $\partial\Omega$ of Ω we need *one* boundary c involving the unknown u. The boundary conditions are of three princip

1. u is prescribed ($u = 0$ or a known time variation for an incoming
2. $\partial u/\partial n = \boldsymbol{n}\cdot\nabla u$ prescribed (zero for reflecting boundaries),
3. an open boundary condition (also called radiation condition) is spe let waves travel undisturbed out of the domain, see Exercise **??** fo

All the listed wave equations with *second-order* derivatives in time n initial conditions:

1. $u = I$,
2. $u_t = V$.

1.2 Mesh

We introduce a mesh in time and in space. The mesh in time consists of time points

$$t_0 = 0 < t_1 < \cdots < t_{N_t},$$

often with a constant spacing $\Delta t = t_{n+1} - t_n$, $n \in \mathcal{I}_t^-$.

Finite difference methods are easy to implement on simple rectangle- or box-shaped domains. More complicated shapes of the domain require substantially more advanced techniques and implementational efforts. On a rectangle- or box-shaped domain mesh points are introduced separately in the various space directions:

$$\begin{aligned} &x_0 < x_1 < \cdots < x_{N_x} \text{ in } x \text{ direction},\\ &y_0 < y_1 < \cdots < y_{N_y} \text{ in } y \text{ direction},\\ &z_0 < z_1 < \cdots < z_{N_z} \text{ in } z \text{ direction}. \end{aligned}$$

We can write a general mesh point as (x_i, y_j, z_k, t_n), with $i \in \mathcal{I}_x$, $j \in \mathcal{I}_y$, $k \in \mathcal{I}_z$, and $n \in \mathcal{I}_t$.

It is a very common choice to use constant mesh spacings: $\Delta x = x_{i+1} - x_i$, $i \in \mathcal{I}_x^-$, $\Delta y = y_{j+1} - y_j$, $j \in \mathcal{I}_y^-$, and $\Delta z = z_{k+1} - z_k$, $k \in \mathcal{I}_z^-$. With equal mesh spacings one often introduces $h = \Delta x = \Delta y = \Delta z$.

The unknown u at mesh point (x_i, y_j, z_k, t_n) is denoted by $u^n_{i,j,k}$. In 2D problems we just skip the z coordinate (by assuming no variation in that direction: $\partial/\partial z = 0$) and write $u^n_{i,j}$.

1.3 Discretization

Two- and three-dimensional wave equations are easily discretized by assembling building blocks for discretization of 1D wave equations, because the multi-dimensional versions just contain terms of the same type that occurs in 1D.

Discretizing the PDEs. Equation (100) can be discretized as

$$[D_t D_t u = c^2(D_x D_x u + D_y D_y u + D_z D_z u) + f]^n_{i,j,k}. \tag{102}$$

The 2D version might be instructive to write out in detail:

$$[D_t D_t u = c^2(D_x D_x u + D_y D_y u) + f]^n_{i,j,k},$$

which becomes

$$\frac{u^{n+1}_{i,j} - 2u^n_{i,j} + u^{n-1}_{i,j}}{\Delta t^2} = c^2 \frac{u^n_{i+1,j} - 2u^n_{i,j} + u^n_{i-1,j}}{\Delta x^2} + c^2 \frac{u^n_{i,j+1} - 2u^n_{i,j} + u^n_{i,j-1}}{\Delta y^2} + f^n_{i,j},$$

Assuming as usual that all values at the time levels n and $n-1$ are kn can solve for the only unknown $u^{n+1}_{i,j}$. The result can be compactly wri

$$u^{n+1}_{i,j} = 2u^n_{i,j} + u^{n-1}_{i,j} + c^2\Delta t^2[D_x D_x u + D_y D_y u]^n_{i,j}.$$

As in the 1D case, we need to develop a special formula for $u^1_{i,j}$ w combine the general scheme for $u^{n+1}_{i,j}$, when $n = 0$, with the discretizatio initial condition:

$$[D_{2t}u = V]^0_{i,j} \quad \Rightarrow \quad u^{-1}_{i,j} = u^1_{i,j} - 2\Delta t V_{i,j}.$$

The result becomes, in compact form,

$$u^{n+1}_{i,j} = u^n_{i,j} - 2\Delta V_{i,j} + \frac{1}{2}c^2\Delta t^2[D_x D_x u + D_y D_y u]^n_{i,j}.$$

The PDE (101) with variable coefficients is discretized term by ter the corresponding elements from the 1D case:

$$[\varrho D_t D_t u = (D_x \overline{q}^x D_x u + D_y \overline{q}^y D_y u + D_z \overline{q}^z D_z u) + f]^n_{i,j,k}.$$

When written out and solved for the unknown $u^{n+1}_{i,j,k}$, one gets the sche

$$\begin{aligned} u^{n+1}_{i,j,k} &= -u^{n-1}_{i,j,k} + 2u^n_{i,j,k} + \\ &= \frac{1}{\varrho_{i,j,k}}\frac{1}{\Delta x^2}(\frac{1}{2}(q_{i,j,k} + q_{i+1,j,k})(u^n_{i+1,j,k} - u^n_{i,j,k}) - \\ &\qquad \frac{1}{2}(q_{i-1,j,k} + q_{i,j,k})(u^n_{i,j,k} - u^n_{i-1,j,k})) + \\ &= \frac{1}{\varrho_{i,j,k}}\frac{1}{\Delta x^2}(\frac{1}{2}(q_{i,j,k} + q_{i,j+1,k})(u^n_{i,j+1,k} - u^n_{i,j,k}) - \\ &\qquad \frac{1}{2}(q_{i,j-1,k} + q_{i,j,k})(u^n_{i,j,k} - u^n_{i,j-1,k})) + \\ &= \frac{1}{\varrho_{i,j,k}}\frac{1}{\Delta x^2}(\frac{1}{2}(q_{i,j,k} + q_{i,j,k+1})(u^n_{i,j,k+1} - u^n_{i,j,k}) - \\ &\qquad \frac{1}{2}(q_{i,j,k-1} + q_{i,j,k})(u^n_{i,j,k} - u^n_{i,j,k-1})) + \\ &+ \qquad \Delta t^2 f^n_{i,j,k}. \end{aligned}$$

Also here we need to develop a special formula for $u^1_{i,j,k}$ by combi scheme for $n = 0$ with the discrete initial condition, which is just a m inserting $u^{-1}_{i,j,k} = u^1_{i,j,k} - 2\Delta t V_{i,j,k}$ in the scheme and solving for $u^1_{i,j,k}$.

Handling boundary conditions where is u known. The scheme above are valid for the internal points in the mesh. After updating t need to visit all the mesh points at the boundaries and set the presc value.

Discretizing the Neumann condition. The condition $\partial u/\partial n = 0$ was implemented in 1D by discretizing it with a $D_{2x}u$ centered difference, and thereafter eliminating the fictitious u point outside the mesh by using the general scheme at the boundary point. Alternatively, one can introduce ghost cells and update the ghost value to for use in the Neumann condition. Exactly the same ideas are used in multi dimensions.

Consider $\partial u/\partial n = 0$ at a boundary $y = 0$. The normal direction is then in the y direction, so

$$\frac{\partial u}{\partial n} = -\frac{\partial u}{\partial y},$$

and we set

$$[-D_{2y}u = 0]^n_{i,0} \quad \Rightarrow \quad \frac{u^n_{i,1} - u^n_{i,-1}}{2\Delta y} = 0\,.$$

From this it follows that $u^n_{i,-1} = u^n_{i,1}$. The discretized PDE at the boundary point $(i, 0)$ reads

$$\frac{u^{n+1}_{i,0} - 2u^n_{i,0} + u^{n-1}_{i,0}}{\Delta t^2} = c^2\frac{u^n_{i+1,0} - 2u^n_{i,0} + u^n_{i-1,0}}{\Delta x^2} + c^2\frac{u^n_{i,1} - 2u^n_{i,0} + u^n_{i,-1}}{\Delta y^2} + f^n_{i,j},$$

We can then just insert $u^1_{i,1}$ for $u^n_{i,-1}$ in this equation and then solve for the boundary value $u^{n+1}_{i,0}$ as done in 1D.

From these calculations, we see a pattern: the general scheme applies at the boundary $j = 0$ too if we just replace $j - 1$ by $j + 1$. Such a pattern is particularly useful for implementations. The details follow from the explained 1D case in Section 6.3.

The alternative approach to eliminating fictitious values outside the mesh is to have $u^n_{i,-1}$ available as a ghost value. The mesh is extended with one extra line (2D) or plane (3D) of ghost cells at a Neumann boundary. In the present example it means that we need a line ghost cells below the y axis. The ghost values must be updated according to $u^{n+1}_{i,-1} = u^{n+1}_{i,1}$.

12.2 Implementation

We shall now describe in detail various Python implementations for solving a standard 2D, linear wave equation with constant wave velocity and $u = 0$ on the boundary. The wave equation is to be solved in the space-time domain $\Omega \times (0, T]$, where $\Omega = (0, L_x) \times (0, L_y)$ is a rectangular spatial domain. More precisely, the complete initial-boundary value problem is defined by

$$u_t = c^2(u_{xx} + u_{yy}) + f(x, y, t), \qquad (x, y) \in \Omega,\ t \in (0, T], \tag{106}$$

$$u(x, y, 0) = I(x, y), \qquad (x, y) \in \Omega, \tag{107}$$

$$u_t(x, y, 0) = V(x, y), \qquad (x, y) \in \Omega, \tag{108}$$

$$u = 0, \qquad (x, y) \in \partial\Omega,\ t \in (0, T], \tag{109}$$

where $\partial\Omega$ is the boundary of Ω, in this case the four sides of the re $[0, L_x] \times [0, L_y]$: $x = 0$, $x = L_x$, $y = 0$, and $y = L_y$.

The PDE is discretized as

$$[D_tD_tu = c^2(D_xD_xu + D_yD_yu) + f]^n_{i,j},$$

which leads to an explicit updating formula to be implemented in a pro

$$u^{n+1} = -u^{n-1}_{i,j} + 2u^n_{i,j} + C^2_x(u^n_{i+1,j} - 2u^n_{i,j} + u^n_{i-1,j}) + C^2_y(u^n_{i,j+1} - 2u^n_{i,j} + u^n_{i,j-1}) + \Delta t$$

for all interior mesh points $i \in \mathcal{I}^i_x$ and $j \in \mathcal{I}^i_y$, and for $n \in \mathcal{I}^+_t$. The co C_x and C_y are defined as

$$C_x = c\frac{\Delta t}{\Delta x}, \quad C_x = c\frac{\Delta t}{\Delta y}\,.$$

At the boundary we simply set $u^{n+1}_{i,j} = 0$ for $i = 0$, $j = 0, \ldots, N_y$; $j = 0, \ldots, N_y$; $j = 0$, $i = 0, \ldots, N_x$; and $j = N_y$, $i = 0, \ldots, N_x$. For t step, $n = 0$, (111) is combined with the discretization of the initial co $u_t = V$, $[D_{2t}u = V]^0_{i,j}$ to obtain a special formula for $u^1_{i,j}$ at the interi points:

$$u^1 = u^0_{i,j} + \Delta t V_{i,j} + \frac{1}{2}C^2_x(u^0_{i+1,j} - 2u^0_{i,j} + u^0_{i-1,j}) + \frac{1}{2}C^2_y(u^0_{i,j+1} - 2u^0_{i,j} + u^0_{i,j-1}) + \frac{1}{2}\Delta$$

The algorithm is very similar to the one in 1D:

1. Set initial condition $u^0_{i,j} = I(x_i, y_j)$
2. Compute $u^1_{i,j}$ from (111)
3. Set $u^1_{i,j} = 0$ for the boundaries $i = 0, N_x$, $j = 0, N_y$
4. For $n = 1, 2, \ldots, N_t$:
   (a) Find $u^{n+1}_{i,j}$ from (111) for all internal mesh points, $i \in \mathcal{I}^i_x$, j
   (b) Set $u^{n+1}_{i,j} = 0$ for the boundaries $i = 0, N_x$, $j = 0, N_y$

12.1 Scalar computations

The `solver` function for a 2D case with constant wave velocity and u boundary condition follows the setup from the similar function for the in `wave1D_u0.py`, but there are a few necessary extensions. The code i program `wave2D_u0.py`[17].

[17] `http://tinyurl.com/nm5587k/wave/wave2D_u0/wave2D_u0.py`

Domain and mesh. The spatial domain is now $[0, L_x] \times [0, L_y]$, specified by the arguments `Lx` and `Ly`. Similarly, the number of mesh points in the x and y directions, N_x and N_y, become the arguments `Nx` and `Ny`. In multi-dimensional problems it makes less sense to specify a Courant number as the wave velocity is a vector and the mesh spacings may differ in the various spatial directions. We therefore give Δt explicitly. The signature of the `solver` function is then

```
def solver(I, V, f, c, Lx, Ly, Nx, Ny, dt, T,
           user_action=None, version='scalar'):
```

Key parameters used in the calculations are created as

```
x = linspace(0, Lx, Nx+1)                  # mesh points in x dir
y = linspace(0, Ly, Ny+1)                  # mesh points in y dir
dx = x[1] - x[0]
dy = y[1] - y[0]
Nt = int(round(T/float(dt)))
t = linspace(0, N*dt, N+1)                 # mesh points in time
Cx2 = (c*dt/dx)**2;  Cy2 = (c*dt/dy)**2    # help variables
dt2 = dt**2
```

Solution arrays. We store $u^{n+1}_{i,j}$, $u^n_{i,j}$, and $u^{n-1}_{i,j}$ in three two-dimensional arrays,

```
u   = zeros((Nx+1,Ny+1))   # solution array
u_1 = zeros((Nx+1,Ny+1))   # solution at t-dt
u_2 = zeros((Nx+1,Ny+1))   # solution at t-2*dt
```

where $u^{n+1}_{i,j}$ corresponds to `u[i,j]`, $u^n_{i,j}$ to `u_1[i,j]`, and $u^{n-1}_{i,j}$ to `u_2[i,j]`

Index sets. It is also convenient to introduce the index sets (cf. Section 6.4)

```
Ix = range(0, u.shape[0])
Iy = range(0, u.shape[1])
It = range(0, t.shape[0])
```

Computing the solution. Inserting the initial condition `I` in `u_1` and making a callback to the user in terms of the `user_action` function is a straightforward generalization of the 1D code from Section 1.6:

```
for i in Ix:
    for j in Iy:
        u_1[i,j] = I(x[i], y[j])

if user_action is not None:
    user_action(u_1, x, xv, y, yv, t, 0)
```


The `user_action` function has additional arguments compared to the The arguments `xv` and `yv` fact will be commented upon in Section 12.2

The key finite difference formula (103) for updating the solution at level is implemented in a separate function as

```
def advance_scalar(u, u_1, u_2, f, x, y, t, n, Cx2, Cy2, dt2,
                   V=None, step1=False):
    Ix = range(0, u.shape[0]);  Iy = range(0, u.shape[1])
    if step1:
        dt = sqrt(dt2)  # save
        Cx2 = 0.5*Cx2;  Cy2 = 0.5*Cy2; dt2 = 0.5*dt2  # redefine
        D1 = 1;  D2 = 0
    else:
        D1 = 2;  D2 = 1
    for i in Ix[1:-1]:
        for j in Iy[1:-1]:
            u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
            u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
            u[i,j] = D1*u_1[i,j] - D2*u_2[i,j] + \
                     Cx2*u_xx + Cy2*u_yy + dt2*f(x[i], y[j], t[n]
            if step1:
                u[i,j] += dt*V(x[i], y[j])
    # Boundary condition u=0
    j = Iy[0]
    for i in Ix: u[i,j] = 0
    j = Iy[-1]
    for i in Ix: u[i,j] = 0
    i = Ix[0]
    for j in Iy: u[i,j] = 0
    i = Ix[-1]
    for j in Iy: u[i,j] = 0
    return u
```

The `step1` variable has been introduced to allow the formula to be re first step $u^1_{i,j}$:

```
u = advance_scalar(u, u_1, u_2, f, x, y, t,
                   n, Cx2, Cy2, dt, V, step1=True)
```

Below, we will make many alternative implementations of the `advance_` function to speed up the code since most of the CPU time in simulations in this function.

12.2 Vectorized computations

The scalar code above turns out to be extremely slow for large 2D mesh probably useless in 3D beyond debugging of small test cases. Vectoriz therefore a must for multi-dimensional finite difference computations in For example, with a mesh consisting of 30×30 cells, vectorization brin the CPU time by a factor of 70 (!).

In the vectorized case we must be able to evaluate user-given functi $I(x, y)$ and $f(x, y, t)$, provided as Python functions `I(x,y)` and `f(x,y` the entire mesh in one array operation. Having the one-dimensional coo arrays `x` and `y` is not sufficient: these must be extended to vectorized v

```
from numpy import newaxis
xv = x[:,newaxis]
yv = y[newaxis,:]
# or
xv = x.reshape((x.size, 1))
yv = y.reshape((1, y.size))
```

his is a standard required technique when evaluating functions over a 2D mesh, ay `sin(xv)*cos(xv)`, which then gives a result with shape `(Nx+1,Ny+1)`.

With the `xv` and `yv` arrays for vectorized computing, setting the initial ondition is just a matter of

```
u_1[:,:] = I(xv, yv)
```

ne could also have written `u_1 = I(xv, yv)` and let `u_1` point to a new object, ut vectorized operations often makes use of direct insertion in the original array rough `u_1[:,:]` because sometimes not all of the array is to be filled by such function evaluation. This is the case with the computational scheme for $u_{i,j}^{n+1}$:

```
def advance_vectorized(u, u_1, u_2, f_a, Cx2, Cy2, dt2,
                       V=None, step1=False):
    if step1:
        dt = sqrt(dt2)  # save
        Cx2 = 0.5*Cx2;  Cy2 = 0.5*Cy2; dt2 = 0.5*dt2  # redefine
        D1 = 1;  D2 = 0
    else:
        D1 = 2;  D2 = 1
    u_xx = u_1[:-2,1:-1] - 2*u_1[1:-1,1:-1] + u_1[2:,1:-1]
    u_yy = u_1[1:-1,:-2] - 2*u_1[1:-1,1:-1] + u_1[1:-1,2:]
    u[1:-1,1:-1] = D1*u_1[1:-1,1:-1] - D2*u_2[1:-1,1:-1] + \
                   Cx2*u_xx + Cy2*u_yy + dt2*f_a[1:-1,1:-1]
    if step1:
        u[1:-1,1:-1] += dt*V[1:-1, 1:-1]
    # Boundary condition u=0
    j = 0
    u[:,j] = 0
    j = u.shape[1]-1
    u[:,j] = 0
    i = 0
    u[i,:] = 0
    i = u.shape[0]-1
    u[i,:] = 0
    return u
```

Array slices in 2D are more complicated to understand than those in 1D, but ıe logic from 1D applies to each dimension separately. For example, when doing $^n_{i,j} - u^n_{i-1,j}$ for $i \in \mathcal{I}_x^+$, we just keep `j` constant and make a slice in the first ıdex: `u_1[1:,j] - u_1[:-1,j]`, exactly as in 1D. The `1:` slice specifies all ıe indices $i = 1, 2, \ldots, N_x$ (up to the last valid index), while `:-1` specifies the elevant indices for the second term: $0, 1, \ldots, N_x - 1$ (up to, but not including ıe last index).

In the above code segment, the situation is slightly more complicated, because ach displaced slice in one direction is accompanied by a `1:-1` slice in the other

direction. The reason is that we only work with the internal points for tl that is kept constant in a difference.

The boundary conditions along the four sides makes use of a slice co of all indices along a boundary:

```
u[: ,0] = 0
u[:,Ny] = 0
u[0 ,:] = 0
u[Nx,:] = 0
```

The `f` function is in the above vectorized update of `u` first compute array over all mesh points:

```
f_a = f(xv, yv, t[n])
```

We could, alternatively, used the call `f(xv, yv, t[n])[1:-1,1:-1]` in term of the update statement, but other implementations in compiled la benefit from having `f` available in an array rather than calling our function `f(x,y,t)` for every point.

Also in the `advance_vectorized` function we have introduced a `step1` to reuse the formula for the first time step in the same way as with `advance_scalar`. We refer to the `solver` function in `wave2D_u0` the details on how the overall algorithm is implemented.

The callback function now has the arguments `u, x, xv, y, yv`. The inclusion of `xv` and `yv` makes it easy to, e.g., compute an exact lution in the callback function and compute errors, through an expres `u - u_exact(xv, yv, t[n])`.

12.3 Verification

Testing a quadratic solution. The 1D solution from Section 2.4 generalized to multi-dimensions and provides a test case where the exact also fulfills the discrete equations such that we know (to machine pr what numbers the solver function should produce. In 2D we use the fo generalization of (30):

$$u_{\mathrm{e}}(x, y, t) = x(L_x - x)y(L_y - y)(1 + \frac{1}{2}t)\,.$$

This solution fulfills the PDE problem if $I(x, y) = u_{\mathrm{e}}(x, y, 0)$, $V = \frac{1}{2}u_{\mathrm{e}}$ and $f = 2c^2(1 + \frac{1}{2}t)(y(L_y - y) + x(L_x - x))$. To show that u_{e} also so discrete equations, we start with the general results $[D_tD_t1]^n = 0$, $[D_tD$ and $[D_tD_tt^2] = 2$, and use these to compute

$$[D_xD_xu_{\mathrm{e}}]^n_{i,j} = [y(L_y - y)(1 + \frac{1}{2}t)D_xD_xx(L_x - x)]^n_{i,j} = y_j(L_y - y_j)(1 +$$

A similar calculation must be carried out for the $[D_yD_yu_{\mathrm{e}}]^n_{i,j}$ and $[D_t$ terms. One must also show that the quadratic solution fits the special

or $u^1_{i,j}$. The details are left as Exercise 11. The `test_quadratic` function in ne `wave2D_u0.py`[18] program implements this verification as a nose test.

.3 Migrating loops to Cython

lthough vectorization can bring down the CPU time dramatically compared with calar code, there is still some factor 5-10 to win in these types of applications by nplementing the finite difference scheme in compiled code, typically in Fortran, , or C++. This can quite easily be done by adding a little extra code to our rogram. Cython is an extension of Python that offers the easiest way to nail ur Python loops in the scalar code down to machine code and the efficiency of .

Cython can be viewed as an extended Python language where variables are eclared with types and where functions are marked to be implemented in C. Migrating Python code to Cython is done by copying the desired code segments o functions (or classes) and placing them in one or more separate files with xtension `.pyx`.

3.1 Declaring variables and annotating the code

Our starting point is the plain `advance_scalar` function for a scalar implementation of the updating algorithm for new values $u^{n+1}_{i,j}$:

```
def advance_scalar(u, u_1, u_2, f, x, y, t, n, Cx2, Cy2, dt2,
                   V=None, step1=False):
    Ix = range(0, u.shape[0]);  Iy = range(0, u.shape[1])
    if step1:
        dt = sqrt(dt2)  # save
        Cx2 = 0.5*Cx2;  Cy2 = 0.5*Cy2; dt2 = 0.5*dt2  # redefine
        D1 = 1;  D2 = 0
    else:
        D1 = 2;  D2 = 1
    for i in Ix[1:-1]:
        for j in Iy[1:-1]:
            u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
            u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
            u[i,j] = D1*u_1[i,j] - D2*u_2[i,j] + \
                     Cx2*u_xx + Cy2*u_yy + dt2*f(x[i], y[j], t[n])
            if step1:
                u[i,j] += dt*V(x[i], y[j])
    # Boundary condition u=0
    j = Iy[0]
    for i in Ix: u[i,j] = 0
    j = Iy[-1]
    for i in Ix: u[i,j] = 0
    i = Ix[0]
    for j in Iy: u[i,j] = 0
    i = Ix[-1]
    for j in Iy: u[i,j] = 0
    return u
```

[18] http://tinyurl.com/nm5587k/wave/wave2D_u0/wave2D_u0.py

We simply take a copy of this function and put it in a file `wave2D_u0_1` The relevant Cython implementation arises from declaring variables wit and adding some important annotations to speed up array computing in Let us first list the complete code in the `.pyx` file:

```
import numpy as np
cimport numpy as np
cimport cython
ctypedef np.float64_t DT    # data type

@cython.boundscheck(False)  # turn off array bounds check
@cython.wraparound(False)   # turn off negative indices (u[-1,-1
cpdef advance(
    np.ndarray[DT, ndim=2, mode='c'] u,
    np.ndarray[DT, ndim=2, mode='c'] u_1,
    np.ndarray[DT, ndim=2, mode='c'] u_2,
    np.ndarray[DT, ndim=2, mode='c'] f,
    double Cx2, double Cy2, double dt2):

    cdef:
        int Ix_start = 0
        int Iy_start = 0
        int Ix_end = u.shape[0]-1
        int Iy_end = u.shape[1]-1
        int i, j
        double u_xx, u_yy

    for i in range(Ix_start+1, Ix_end):
        for j in range(Iy_start+1, Iy_end):
            u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
            u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
            u[i,j] = 2*u_1[i,j] - u_2[i,j] + \
                     Cx2*u_xx + Cy2*u_yy + dt2*f[i,j]
    # Boundary condition u=0
    j = Iy_start
    for i in range(Ix_start, Ix_end+1): u[i,j] = 0
    j = Iy_end
    for i in range(Ix_start, Ix_end+1): u[i,j] = 0
    i = Ix_start
    for j in range(Iy_start, Iy_end+1): u[i,j] = 0
    i = Ix_end
    for j in range(Iy_start, Iy_end+1): u[i,j] = 0
    return u
```

This example may act as a recipe on how to transform array-intensi with loops into Cython.

1. Variables are declared with types: for example, `double v` in the a list instead of just `v`, and `cdef double v` for a variable `v` in the the function. A Python `float` object is declared as `double` for tra to C by Cython, while an `int` object is declared by `int`.

2. Arrays need a comprehensive type declaration involving

   - the type `np.ndarray`,
   - the data type of the elements, here 64-bit floats, abbreviate through `ctypedef np.float64_t DT` (instead of `DT` we could

full name of the data type: `np.float64_t`, which is a Cython-defined type),

- the dimensions of the array, here `ndim=2` and `ndim=1`,
- specification of contiguous memory for the array (`mode='c'`).

3. Functions declared with `cpdef` are translated to C but also accessible from Python.

4. In addition to the standard `numpy` import we also need a special Cython import of `numpy`: `cimport numpy as np`, to appear *after* the standard import.

5. By default, array indices are checked to be within their legal limits. To speed up the code one should turn off this feature for a specific function by placing `@cython.boundscheck(False)` above the function header.

6. Also by default, array indices can be negative (counting from the end), but this feature has a performance penalty and is therefore here turned off by writing `@cython.wraparound(False)` right above the function header.

7. The use of index sets `Ix` and `Iy` in the scalar code cannot be successfully translated to C. One reason is that constructions like `Ix[1:-1]` involve negative indices, and these are now turned off. Another reason is that Cython loops must take the form `for i in xrange` or `for i in range` for being translated into efficient C loops. We have therefore introduced `Ix_start` as `Ix[0]` and `Ix_end` as `Ix[-1]` to hold the start and end of the values of index i. Similar variables are introduced for the j index. A loop `for i in Ix` is with these new variables written as `for i in range(Ix_start, Ix_end+1)`.

Array declaration syntax in Cython.

We have used the syntax `np.ndarray[DT, ndim=2, mode='c']` to declare `numpy` arrays in Cython. There is a simpler, alternative syntax, employing typed memory views[a], where the declaration looks like `double [:,:]`. However, the full support for this functionality is not yet ready, and in this text we use the full array declaration syntax.

[a] `http://docs.cython.org/src/userguide/memoryviews.html`

3.2 Visual inspection of the C translation

ython can visually explain how successfully it can translate a code from Python
C. The command


```
Terminal> cython -a wave2D_u0_loop_cy.pyx
```

produces an HTML file `wave2D_u0_loop_cy.html`, which can be loade
web browser to illustrate which lines of the code that have been translat
Figure 8 shows the illustrated code. Yellow lines indicate the lines that
did not manage to translate to efficient C code and that remain in Pyth
the present code we see that Cython is able to translate all the loops wi
computing to C, which is our primary goal.

Raw output: wave2D_u0_loop_cy.c

```
1: import numpy as np
2: cimport numpy as np
3: cimport cython
4: ctypedef np.float64_t DT    # data type
5:
6: @cython.boundscheck(False)  # turn off array bounds check
7: @cython.wraparound(False)   # turn off negative indices (u[-1,-1])
8: cpdef advance(
9:     np.ndarray[DT, ndim=2, mode='c'] u,
10:     np.ndarray[DT, ndim=2, mode='c'] u_1,
11:     np.ndarray[DT, ndim=2, mode='c'] u_2,
12:     np.ndarray[DT, ndim=2, mode='c'] f,
13:     double Cx2, double Cy2, double dt2):
14:
15:     cdef int Ix_start = 0
16:     cdef int Iy_start = 0
17:     cdef int Ix_end = u.shape[0]-1
18:     cdef int Iy_end = u.shape[1]-1
19:     cdef int i, j
20:     cdef double u_xx, u_yy
21:
22:     for i in range(Ix_start+1, Ix_end):
23:         for j in range(Iy_start+1, Iy_end):
24:             u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
25:             u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
26:             u[i,j] = 2*u_1[i,j] - u_2[i,j] + \
27:                      Cx2*u_xx + Cy2*u_yy + dt2*f[i,j]
28:     # Boundary condition u=0
29:     j = Iy_start
30:     for i in range(Ix_start, Ix_end+1): u[i,j] = 0
31:     j = Iy_end
32:     for i in range(Ix_start, Ix_end+1): u[i,j] = 0
33:     i = Ix_start
34:     for j in range(Iy_start, Iy_end+1): u[i,j] = 0
35:     i = Iy_end
36:     for j in range(Iy_start, Iy_end+1): u[i,j] = 0
37:     return u
```

Figure 8: Visual illustration of Cython's ability to translate Python

You can also inspect the generated C code directly, as it appears in
`wave2D_u0_loop_cy.c`. Nevertheless, understanding this C code requir
familiarity with writing Python extension modules in C by hand. Deep
the file we can see in detail how the compute-intensive statements are tra
some complex C code that is quite different from what we a human wou
(at least if a direct correspondence to the mathematics was in mind).

13.3 Building the extension module

Cython code must be translated to C, compiled, and linked to form what i
in the Python world as a *C extension module*. This is usually done by m
`setup.py` script, which is the standard way of building and installing
software. For an extension module arising from Cython code, the fo
`setup.py` script is all we need to build and install the module:

```
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext

cymodule = 'wave2D_u0_loop_cy'
```

```
setup(
  name=cymodule
  ext_modules=[Extension(cymodule, [cymodule + '.pyx'],)],
  cmdclass={'build_ext': build_ext},
)
```

We run the script by

```
Terminal> python setup.py build_ext --inplace
```

The `-inplace` option makes the extension module available in the current directory as the file `wave2D_u0_loop_cy.so`. This file acts as a normal Python module that can be imported and inspected:

```
>>> import wave2D_u0_loop_cy
>>> dir(wave2D_u0_loop_cy)
['__builtins__', '__doc__', '__file__', '__name__',
 '__package__', '__test__', 'advance', 'np']
```

The important output from the `dir` function is our Cython function `advance` the module also features the imported `numpy` module under the name `np` as well as many standard Python objects with double underscores in their names).

The `setup.py` file makes use of the `distutils` package in Python and Cython's extension of this package. These tools know how Python was built on the computer and will use compatible compiler(s) and options when building other code in Cython, C, or C++. Quite some experience with building large program systems is needed to do the build process manually, so using a `setup.py` script is strongly recommended.

Simplified build of a Cython module.

When there is no need to link the C code with special libraries, Cython offers a shortcut for generating and importing the extension module:

```
import pyximport; pyximport.install()
```

This makes the `setup.py` script redundant. However, in the `wave2D_u0.py` code we do not use `pyximport` and require an explicit build process of this and many other modules.

3.4 Calling the Cython function from Python

The `wave2D_u0_loop_cy` module contains our `advance` function, which we now may call from the Python program for the wave equation:


```
import wave2D_u0_loop_cy
advance = wave2D_u0_loop_cy.advance
...
for n in It[1:-1:                    # time loop
    f_a[:,:] = f(xv, yv, t[n])     # precompute, size as u
    u = advance(u, u_1, u_2, f_a, x, y, t, Cx2, Cy2, dt2)
```

Efficiency. For a mesh consisting of 120×120 cells, the scalar Pyth require 1370 CPU time units, the vectorized version requires 5.5, w Cython version requires only 1! For a smaller mesh with 60×60 cells C about 1000 times faster than the scalar Python code, and the vectorized is about 6 times slower than the Cython version.

14 Migrating loops to Fortran

Instead of relying on Cython's (excellent) ability to translate Python t can invoke a compiled language directly and write the loops ourselves. start with Fortran 77, because this is a language with more convenier handling than C (or plain C++). Or more precisely, we can with ease p with the same multi-dimensional indices in the Fortran code as in th arrays in the Python code, while in C these arrays are one-dimensio requires us to reduce multi-dimensional indices to a single index.

14.1 The Fortran subroutine

We write a Fortran subroutine `advance` in a file `wave2D_u0_loop_f77` implementing the updating formula (111) and setting the solution to zer boundaries:

```
      subroutine advance(u, u_1, u_2, f, Cx2, Cy2, dt2, Nx, Ny)
      integer Nx, Ny
      real*8 u(0:Nx,0:Ny), u_1(0:Nx,0:Ny), u_2(0:Nx,0:Ny)
      real*8 f(0:Nx,0:Ny), Cx2, Cy2, dt2
      integer i, j
      real*8 u_xx, u_yy
Cf2py intent(in, out) u

C     Scheme at interior points
      do j = 1, Ny-1
         do i = 1, Nx-1
            u_xx = u_1(i-1,j) - 2*u_1(i,j) + u_1(i+1,j)
            u_yy = u_1(i,j-1) - 2*u_1(i,j) + u_1(i,j+1)
            u(i,j) = 2*u_1(i,j) - u_2(i,j) + Cx2*u_xx + Cy2*u_yy
     &               dt2*f(i,j)
         end do
      end do

C     Boundary conditions
```

[19] http://tinyurl.com/nm5587k/wave/wave2D_u0/wave2D_u0_loop_f77.f

```
      j = 0
      do i = 0, Nx
         u(i,j) = 0
      end do
      j = Ny
      do i = 0, Nx
         u(i,j) = 0
      end do
      i = 0
      do j = 0, Ny
         u(i,j) = 0
      end do
      i = Nx
      do j = 0, Ny
         u(i,j) = 0
      end do
      return
      end
```

his code is plain Fortran 77, except for the special `Cf2py` comment line, which ere specifies that `u` is both an input argument *and* an object to be returned om the `advance` routine. Or more precisely, Fortran is not able return an array om a function, but we need a *wrapper code* in C for the Fortran subroutine to nable calling it from Python, and in this wrapper code one can return `u` to the alling Python code.

Remark.

It is not strictly necessary to return `u` to the calling Python code since the `advance` function will modify the elements of `u`, but the convention in Python is to get all output from a function as returned values. That is, the right way of calling the above Fortran subroutine from Python is

```
u = advance(u, u_1, u_2, f, Cx2, Cy2, dt2)
```

The less encouraged style, which works and resembles the way the Fortran subroutine is called from Fortran, reads

```
advance(u, u_1, u_2, f, Cx2, Cy2, dt2)
```

4.2 Building the Fortran module with f2py

he nice feature of writing loops in Fortran is that the tool `f2py` can with very ttle work produce a C extension module such that we can call the Fortran ersion of `advance` from Python. The necessary commands to run are


```
Terminal> f2py -m wave2D_u0_loop_f77 -h wave2D_u0_loop_f77.pyf \
          --overwrite-signature wave2D_u0_loop_f77.f
Terminal> f2py -c wave2D_u0_loop_f77.pyf --build-dir build_f77 \
          -DF2PY_REPORT_ON_ARRAY_COPY=1 wave2D_u0_loop_f77.f
```

The first command asks `f2py` to interpret the Fortran code and make a Fo specification of the extension module in the file `wave2D_u0_loop_f77.p` second command makes `f2py` generate all necessary wrapper code, com Fortran file and the wrapper code, and finally build the module. The build takes place in the specified subdirectory `build_f77` so that files can be ir if something goes wrong. The option `-DF2PY_REPORT_ON_ARRAY_COPY=` `f2py` write a message for every array that is copied in the communication Fortran and Python, which is very useful for avoiding unnecessary array (see below). The name of the module file is `wave2D_u0_loop_f77.so`, file can be imported and inspected as any other Python module:

```
>>> import wave2D_u0_loop_f77
>>> dir(wave2D_u0_loop_f77)
['__doc__', '__file__', '__name__', '__package__',
 '__version__', 'advance']
>>> print wave2D_u0_loop_f77.__doc__
This module 'wave2D_u0_loop_f77' is auto-generated with f2py....
Functions:
  u = advance(u,u_1,u_2,f,cx2,cy2,dt2,
      nx=(shape(u,0)-1),ny=(shape(u,1)-1))
```

Examine the doc strings!

Printing the doc strings of the module and its functions is extre important after having created a module with `f2py`, because `f2py` n Python interfaces to the Fortran functions that are different from the functions are declared in the Fortran code (!). The rationale fo behavior is that `f2py` creates *Pythonic* interfaces such that Fortran rou can be called in the same way as one calls Python functions. Output from Python functions is always returned to the calling code, but t technically impossible in Fortran. Also, arrays in Python are pass Python functions without their dimensions because that informati packed with the array data in the array objects, but this is not pos in Fortran. Therefore, `f2py` removes array dimensions from the argu list, and `f2py` makes it possible to return objects back to Python.

Let us follow the advice of examining the doc strings and take a cl at the documentation `f2py` has generated for our Fortran `advance` sub

```
>>> print wave2D_u0_loop_f77.advance.__doc__
This module 'wave2D_u0_loop_f77' is auto-generated with f2py
Functions:
```

```
  u = advance(u,u_1,u_2,f,cx2,cy2,dt2,
              nx=(shape(u,0)-1),ny=(shape(u,1)-1))

dvance - Function signature:
  u = advance(u,u_1,u_2,f,cx2,cy2,dt2,[nx,ny])
Required arguments:
  u : input rank-2 array('d') with bounds (nx + 1,ny + 1)
  u_1 : input rank-2 array('d') with bounds (nx + 1,ny + 1)
  u_2 : input rank-2 array('d') with bounds (nx + 1,ny + 1)
  f : input rank-2 array('d') with bounds (nx + 1,ny + 1)
  cx2 : input float
  cy2 : input float
  dt2 : input float
Optional arguments:
  nx := (shape(u,0)-1) input int
  ny := (shape(u,1)-1) input int
Return objects:
  u : rank-2 array('d') with bounds (nx + 1,ny + 1)
```

ere we see that the `nx` and `ny` parameters declared in Fortran are optional rguments that can be omitted when calling `advance` from Python.

We strongly recommend to print out the documentation of *every* Fortran nction to be called from Python and make sure the call syntax is exactly as sted in the documentation.

4.3 How to avoid array copying

Iulti-dimensional arrays are stored as a stream of numbers in memory. For two-dimensional array consisting of rows and columns there are two ways f creating such a stream: *row-major ordering*, which means that rows are ored consecutively in memory, or *column-major ordering*, which means that the olumns are stored one after each other. All programming languages inherited om C, including Python, apply the row-major ordering, but Fortran uses olumn-major storage. Thinking of a two-dimensional array in Python or C as a natrix, it means that Fortran works with the transposed matrix.

Fortunately, `f2py` creates extra code so that accessing `u(i,j)` in the Fortran ubroutine corresponds to the element `u[i,j]` in the underlying `numpy` array without the extra code, `u(i,j)` in Fortran would access `u[j,i]` in the `numpy` rray). Technically, `f2py` takes a copy of our `numpy` array and reorders the data efore sending the array to Fortran. Such copying can be costly. For 2D wave mulations on a 60×60 grid the overhead of copying is a factor of 5, which eans that almost the whole performance gain of Fortran over vectorized `numpy` ode is lost!

To avoid having `f2py` to copy arrays with C storage to the corresponding ortran storage, we declare the arrays with Fortran storage:

```
order = 'Fortran' if version == 'f77' else 'C'
u   = zeros((Nx+1,Ny+1), order=order)   # solution array
u_1 = zeros((Nx+1,Ny+1), order=order)   # solution at t-dt
u_2 = zeros((Nx+1,Ny+1), order=order)   # solution at t-2*dt
```


In the compile and build step of using `f2py`, it is recommended to extra option for making `f2py` report on array copying:

```
Terminal> f2py -c wave2D_u0_loop_f77.pyf --build-dir build_f77 \
          -DF2PY_REPORT_ON_ARRAY_COPY=1 wave2D_u0_loop_f77.f
```

It can sometimes be a challenge to track down which array that c copying. There are two principal reasons for copying array data: either t does not have Fortran storage or the element types do not match those in the Fortran code. The latter cause is usually effectively eliminated b `real*8` data in the Fortran code and `float64` (the default `float` type in in the arrays on the Python side. The former reason is more common. check whether an array before a Fortran call has the right storage one c the result of `isfortran(a)`, which is `True` if the array `a` has Fortran st

Let us look at an example where we face problems with array sto typical problem in the `wave2D_u0.py` code is to set

```
f_a = f(xv, yv, t[n])
```

before the call to the Fortran `advance` routine. This computation create array with C storage. An undesired copy of `f_a` will be produced when `f_a` to a Fortran routine. There are two remedies, either direct insertion in an array with Fortran storage,

```
f_a = zeros((Nx+1, Ny+1), order='Fortran')
...
f_a[:,:] = f(xv, yv, t[n])
```

or remaking the `f(xv, yv, t[n])` array,

```
f_a = asarray(f(xv, yv, t[n]), order='Fortran')
```

The former remedy is most efficient if the `asarray` operation is to be pe a large number of times.

Efficiency. The efficiency of this Fortran code is very similar to the code. There is usually nothing more to gain, from a computational ef point of view, by implementing the *complete* Python program in Fortr That will just be a lot more code for all administering work that is ne scientific software, especially if we extend our sample program `wave2D_u` handle a real scientific problem. Then only a small portion will consist with intensive array calculations. These can be migrated to Cython or as explained, while the rest of the programming can be more convenient in Python.

.5 Migrating loops to C via Cython

he computationally intensive loops can alternatively be implemented in C ode. Just as Fortran calls for care regarding the storage of two-dimensional rrays, working with two-dimensional arrays in C is a bit tricky. The reason is iat `numpy` arrays are viewed as one-dimensional arrays when transferred to C, hile C programmers will think of `u`, `u_1`, and `u_2` as two dimensional arrays nd index them like `u[i][j]`. The C code must declare `u` as `double* u` and ranslate an index pair `[i][j]` to a corresponding single index when `u` is viewed s one-dimensional. This translation requires knowledge of how the numbers in are stored in memory.

5.1 Translating index pairs to single indices

wo-dimensional `numpy` arrays with the default C storage are stored row by row. n general, multi-dimensional arrays with C storage are stored such that the last ndex has the fastest variation, then the next last index, and so on, ending up ith the slowest variation in the first index. For a two-dimensional `u` declared s `zeros((Nx+1,Ny+1))` in Python, the individual elements are stored in the llowing order:

```
u[0,0], u[0,1], u[0,2], ..., u[0,Ny], u[1,0], u[1,1], ...,
u[1,Ny], u[2,0], ..., u[Nx,0], u[Nx,1], ..., u[Nx, Ny]
```

Viewing `u` as one-dimensional, the index pair (i, j) translates to $i(N_y + 1) + j$. o, where a C programmer would naturally write an index `u[i][j]`, the indexing ust read `u[i*(Ny+1) + j]`. This is tedious to write, so it can be handy to efine a C macro,

```
#define idx(i,j) (i)*(Ny+1) + j
```

o that we can write `u[idx(i,j)]`, which reads much better and is easier to ebug.

Be careful with macro definitions.

Macros just perform simple text substitutions: `idx(hello,world)` is expanded to `(hello)*(Ny+1) + world`. The parenthesis in `(i)` are essential - using the natural mathematical formula `i*(Ny+1) + j` in the macro definition, `idx(i-1,j)` would expand to `i-1*(Ny+1) + j`, which is the wrong formula. Macros are handy, but requires careful use. In C++, inline functions are safer and replace the need for macros.

5.2 The complete C code

he C version of our function `advance` can be coded as follows.


```
#define idx(i,j) (i)*(Ny+1) + j

void advance(double* u, double* u_1, double* u_2, double* f,
             double Cx2, double Cy2, double dt2, int Nx, int Ny)
{
  int i, j;
  double u_xx, u_yy;
  /* Scheme at interior points */
  for (i=1; i<=Nx-1; i++) {
    for (j=1; j<=Ny-1; j++) {
      u_xx = u_1[idx(i-1,j)] - 2*u_1[idx(i,j)] + u_1[idx(i+1,j)]
      u_yy = u_1[idx(i,j-1)] - 2*u_1[idx(i,j)] + u_1[idx(i,j+1)]
      u[idx(i,j)] = 2*u_1[idx(i,j)] - u_2[idx(i,j)] +
        Cx2*u_xx + Cy2*u_yy + dt2*f[idx(i,j)];
    }
  }
  /* Boundary conditions */
  j = 0;  for (i=0; i<=Nx; i++) u[idx(i,j)] = 0;
  j = Ny; for (i=0; i<=Nx; i++) u[idx(i,j)] = 0;
  i = 0;  for (j=0; j<=Ny; j++) u[idx(i,j)] = 0;
  i = Nx; for (j=0; j<=Ny; j++) u[idx(i,j)] = 0;
}
```

15.3 The Cython interface file

All the code above appears in a file `wave2D_u0_loop_c.c`[20]. We need to this file together with C wrapper code such that `advance` can be call Python. Cython can be used to generate appropriate wrapper code. The Cython code for interfacing C is placed in a file with extension `.pyx`. H file, called `wave2D_u0_loop_c_cy.pyx`[21], looks like

```
import numpy as np
cimport numpy as np
cimport cython

cdef extern from "wave2D_u0_loop_c.h":
    void advance(double* u, double* u_1, double* u_2, double* f,
                 double Cx2, double Cy2, double dt2,
                 int Nx, int Ny)

@cython.boundscheck(False)
@cython.wraparound(False)
def advance_cwrap(
    np.ndarray[double, ndim=2, mode='c'] u,
    np.ndarray[double, ndim=2, mode='c'] u_1,
    np.ndarray[double, ndim=2, mode='c'] u_2,
    np.ndarray[double, ndim=2, mode='c'] f,
    double Cx2, double Cy2, double dt2):
    advance(&u[0,0], &u_1[0,0], &u_2[0,0], &f[0,0],
            Cx2, Cy2, dt2,
            u.shape[0]-1, u.shape[1]-1)
    return u
```

[20] http://tinyurl.com/nm5587k/wave//wave2D_u0/wave2D_u0_loop_c.c
[21] http://tinyurl.com/nm5587k/wave/wave2D_u0/wave2D_u0_loop_c_cy.pyx

/e first declare the C functions to be interfaced. These must also appear in a C eader file, `wave2D_u0_loop_c.h`[22],

```
extern void advance(double* u, double* u_1, double* u_2, double* f,
                    double Cx2, double Cy2, double dt2,
                    int Nx, int Ny);
```

he next step is to write a Cython function with Python objects as arguments. he name `advance` is already used for the C function so the function to be called om Python is named `advance_cwrap`. The contents of this function is simply call to the `advance` version in C. To this end, the right information from the ython objects must be passed on as arguments to `advance`. Arrays are sent ith their C pointers to the first element, obtained in Cython as `&u[0,0]` (the takes the address of a C variable). The `Nx` and `Ny` arguments in `advance` are asily obtained from the shape of the `numpy` array `u`. Finally, `u` must be returned ıch that we can set `u = advance(...)` in Python.

5.4 Building the extension module

remains to build the extension module. An appropriate `setup.py` file is

```
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext

sources = ['wave2D_u0_loop_c.c', 'wave2D_u0_loop_c_cy.pyx']
module = 'wave2D_u0_loop_c_cy'
setup(
  name=module,
  ext_modules=[Extension(module, sources,
                         libraries=[], # C libs to link with
                         )],
  cmdclass={'build_ext': build_ext},
)
```

ll we need to specify is the `.c` file(s) and the `.pyx` interface file. Cython is au- omatically run to generate the necessary wrapper code. Files are then compiled nd linked to an extension module residing in the file `wave2D_u0_loop_c_cy.so`. ere is a session with running `setup.py` and examining the resulting module in ython

```
erminal> python setup.py build_ext --inplace
erminal> python
>> import wave2D_u0_loop_c_cy as m
>> dir(m)
'__builtins__', '__doc__', '__file__', '__name__', '__package__',
'__test__', 'advance_cwrap', 'np']
```

[22] http://tinyurl.com/nm5587k/wave/wave2D_u0/wave2D_u0_loop_c.h

The call to the C version of `advance` can go like this in Python:

```
import wave2D_u0_loop_c_cy
advance = wave2D_u0_loop_c_cy.advance_cwrap
...
f_a[:,:] = f(xv, yv, t[n])
u = advance(u, u_1, u_2, f_a, Cx2, Cy2, dt2)
```

Efficiency. In this example, the C and Fortran code runs at the sam and there are no significant differences in the efficiency of the wrapper co overhead implied by the wrapper code is negligible as long as we do n with very small meshes and consequently little numerical work in the a function.

16 Migrating loops to C via f2py

An alternative to using Cython for interfacing C code is to apply `f2py` code is the same, just the details of specifying how it is to be called from differ. The `f2py` tool requires the call specification to be a Fortran 90 defined in a `.pyf` file. This file was automatically generated when we in a Fortran subroutine. With a C function we need to write this module o or we can use a trick and let `f2py` generate it for us. The trick consists in the signature of the C function with Fortran syntax and place it in a file, here `wave2D_u0_loop_c_f2py_signature.f`:

```
      subroutine advance(u, u_1, u_2, f, Cx2, Cy2, dt2, Nx, Ny)
Cf2py intent(c) advance
      integer Nx, Ny, N
      real*8 u(0:Nx,0:Ny), u_1(0:Nx,0:Ny), u_2(0:Nx,0:Ny)
      real*8 f(0:Nx, 0:Ny), Cx2, Cy2, dt2
Cf2py intent(in, out) u
Cf2py intent(c) u, u_1, u_2, f, Cx2, Cy2, dt2, Nx, Ny
      return
      end
```

Note that we need a special `f2py` instruction, through a `Cf2py` comment telling that all the function arguments are C variables. We also need to that the function is actually in C: `intent(c) advance`.

Since `f2py` is just concerned with the function signature and not the c contents of the function body, it can easily generate the Fortran 90 specification based solely on the signature above:

```
Terminal> f2py -m wave2D_u0_loop_c_f2py \
          -h wave2D_u0_loop_c_f2py.pyf --overwrite-signature \
          wave2D_u0_loop_c_f2py_signature.f
```

he compile and build step is as for the Fortran code, except that we list C files ıstead of Fortran files:

```
erminal> f2py -c wave2D_u0_loop_c_f2py.pyf \
         --build-dir tmp_build_c \
         -DF2PY_REPORT_ON_ARRAY_COPY=1 wave2D_u0_loop_c.c
```

s when interfacing Fortran code with `f2py`, we need to print out the doc string ɔ see the exact call syntax from the Python side. This doc string is identical ɔr the C and Fortran versions of `advance`.

6.1 Migrating loops to C++ via f2py

++ is a much more versatile language than C or Fortran and has over the last vo decades become very popular for numerical computing. Many will therefore refer to migrate compute-intensive Python code to C++. This is, in principle, ısy: just write the desired C++ code and use some tool for interfacing it ɔm Python. A tool like SWIG[23] can interpret the C++ code and generate ıterfaces for a wide range of languages, including Python, Perl, Ruby, and Java. owever, SWIG is a comprehensive tool with a correspondingly steep learning ırve. Alternative tools, such as Boost Python[24], SIP[25], and Shiboken[26] are milarly comprehensive. Simpler tools include PyBindGen[27],

A technically much easier way of interfacing C++ code is to drop the ossibility to use C++ classes directly from Python, but instead make a C ıterface to the C++ code. The C interface can be handled by `f2py` as shown ı the example with pure C code. Such a solution means that classes in Python nd C++ cannot be mixed and that only primitive data types like numbers, rings, and arrays can be transferred between Python and C++. Actually, this often a very good solution because it forces the C++ code to work on array ata, which usually gives faster code than if fancy data structures with classes re used. The arrays coming from Python, and looking like plain C/C++ arrays, ın be efficiently wrapped in more user-friendly C++ array classes in the C++ ɔde, if desired.

7 Using classes to implement a simulator

- Introduce classes `Mesh`, `Function`, `Problem`, `Solver`, `Visualizer`, `File`

[23] http://swig.org/
[24] http://www.boost.org/doc/libs/1_51_0/libs/python/doc/index.html
[25] http://riverbankcomputing.co.uk/software/sip/intro
[26] http://qt-project.org/wiki/Category:LanguageBindings::PySide::Shiboken
[27] http://code.google.com/p/pybindgen/

18 Exercises

Exercise 11: Check that a solution fulfills the discrete

Carry out all mathematical details to show that (112) is indeed a sol the discrete model for a 2D wave equation with $u = 0$ on the bounda must check the boundary conditions, the initial conditions, the general equation at a time level and the special version of this equation for the fi level. Filename: `check_quadratic_solution.pdf`.

Project 12: Calculus with 2D/3D mesh functions

The goal of this project is to redo Project 5 with 2D and 3D mesh fu ($f_{i,j}$ and $_{fi,j,k}$).

Differentiation. The differentiation results in a discrete gradient f which in the 2D case can be represented by a three-dimensional array `df[` where `d` represents the direction of the derivative and `i` and `j` are mes counters in 2D (the 3D counterpart is `df[d,i,j,k]`).

Integration. The integral of a 2D mesh function $f_{i,j}$ is defined as

$$F_{i,j} = \int_{y_0}^{y_j}\int_{x_0}^{x_i} f(x,y)dxdy,$$

where $f(x,y)$ is a function that takes on the values of the discrete mesh f $f_{i,j}$ at the mesh points, but can also be evaluated in between the mesh The particular variation between mesh points can be taken as bilinear, is not important as we will use a product Trapezoidal rule to approxim integral over a cell in the mesh and then we only need to evaluate $f(x,y$ mesh points.

Suppose $F_{i,j}$ is computed. The calculation of $F_{i+1,j}$ is then

$$\begin{aligned} F_{i+1,j} &= F_{i,j} + \int_{x_i}^{x_{i+1}}\int_{y_0}^{y_j} f(x,y)dydx \\ &\approx \Delta x \int_{y_0}^{y_j} f(x_{i+\frac{1}{2}},y)dy \\ &\approx \Delta x \frac{1}{2}\left(\int_{y_0}^{y_j} f(x_i,y)dy + \int_{y_0}^{y_j} f(x_{i+1},y)dy\right) \end{aligned}$$

The integrals in the y direction can be approximated by a Trapezoidal similar idea can be used to compute $F_{i,j+1}$. Thereafter, $F_{i+1,j+1}$ can be cc by adding the integral over the final corner cell to $F_{i+1,j} + F_{i,j+1} - F_{i,j}$ out the details of these computations and extend the ideas to 3D. Fi `mesh_calculus_3D.py`.

Exercise 13: Implement Neumann conditions in 2D

Modify the `wave2D_u0.py`[28] program, which solves the 2D wave equation $u_{tt} = c^2(u_{xx} + u_{yy})$ with constant wave velocity c and $u = 0$ on the boundary, to have Neumann boundary conditions: $\partial u/\partial n = 0$. Include both scalar code (for debugging and reference) and vectorized code (for speed).

To test the code, use $u = 1.2$ as solution ($I(x, y) = 1.2$, $V = f = 0$, and c arbitrary), which should be exactly reproduced with any mesh as long as the stability criterion is satisfied. Another test is to use the plug-shaped pulse in the `pulse` function from Section 8 and the `wave1D_dn_vc.py`[29] program. This pulse is exactly propagated in 1D if $c\Delta t/\Delta x = 1$. Check that also the 2D program can propagate this pulse exactly in x direction ($c\Delta t/\Delta x = 1$, Δy arbitrary) and y direction ($c\Delta t/\Delta y = 1$, Δx arbitrary). Filename: `wave2D_dn.py`.

Exercise 14: Test the efficiency of compiled loops in 3D

Extend the `wave2D_u0.py` code and the Cython, Fortran, and C versions to 3D. Set up an efficiency experiment to determine the relative efficiency of pure scalar Python code, vectorized code, Cython-compiled loops, Fortran-compiled loops, and C-compiled loops. Normalize the CPU time for each mesh by the fastest version. Filename: `wave3D_u0.py`.

9 Applications of wave equations

This section presents a range of wave equation models for different physical phenomena. Although many wave motion problems in physics can be modeled by the standard linear wave equation, or a similar formulation with a system of first-order equations, there are some exceptions. Perhaps the most important is water waves: these are modeled by the Laplace equation with time-dependent boundary conditions at the water surface (long water waves, however, can be approximated by a standard wave equation, see Section 19.7). Quantum mechanical waves constitute another example where the waves are governed by the Schrödinger equation and not a standard wave equation. Many wave phenomena also need to take nonlinear effects into account when the wave amplitude is significant. Shock waves in the air is a primary example.

The derivations in the following are very brief. Those with a firm background in continuum mechanics will probably have enough information to fill in the details, while other readers will hopefully get some impression of the physics and approximations involved when establishing wave equation models.

9.1 Waves on a string

Figure 9 shows a model we may use to derive the equation for waves on a string. The string is modeled as a set of discrete point masses (at mesh points) with

[28] `http://tinyurl.com/nm5587k/wave/wave2D_u0/wave2D_u0.py`
[29] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_dn_vc.py`

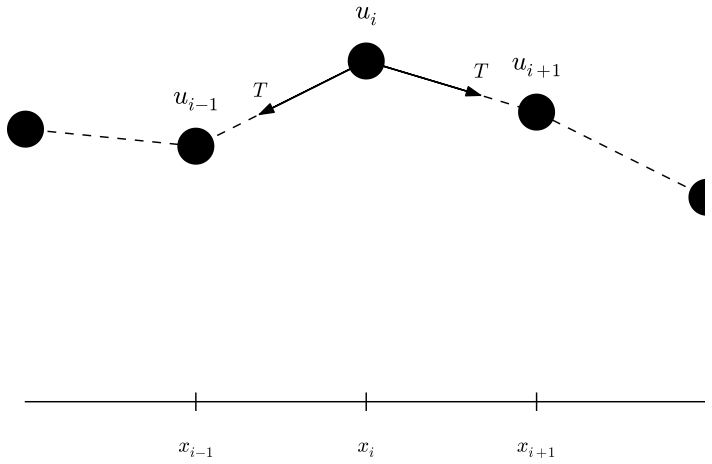


Figure 9: Discrete string model with point masses connected by elastic s

elastic strings in between. The strings are at a high constant tension let the mass at mesh point x_i be m_i. The displacement of this mass pc direction is denoted by $u_i(t)$.

The motion of mass m_i is governed by Newton's second law of moti position of the mass at time t is $x_i\boldsymbol{i} + u_i(t)\boldsymbol{j}$, where $\boldsymbol{i}$ and $\boldsymbol{j}$ are unit ve the x and y direction, respectively. The acceleration is then $u_i''(t)\boldsymbol{j}$. Tw are acting on the mass as indicated in Figure 9. The force $\boldsymbol{T}^-$ acting tov point x_{i-1} can be decomposed as

$$\boldsymbol{T}^- = -T\sin\phi\boldsymbol{i} - T\cos\phi\boldsymbol{j},$$

where ϕ is the angle between the force and the line $x = x_i$. Let $\Delta u_i = u$ and let $\Delta s_i = \sqrt{\Delta u_i^2 + (x_i - x_{i-1})^2}$ be the distance from mass m_{i-1}

$_i$. It is seen that $\cos\phi = \Delta u_i/\Delta s_i$ and $\sin\phi = (x_i - x_{i-1})/\Delta s$ or $\Delta x/\Delta s_i$ if e introduce a constant mesh spacing $\Delta x = x_i - x_{i-1}$. The force can then be ritten

$$\boldsymbol{T}^- = -T\frac{\Delta x}{\Delta s_i}\boldsymbol{i} - T\frac{\Delta u_i}{\Delta s_i}\boldsymbol{j}\,.$$

he force $\boldsymbol{T}^+$ acting toward x_{i+1} can be calculated in a similar way:

$$\boldsymbol{T}^+ = T\frac{\Delta x}{\Delta s_{i+1}}\boldsymbol{i} + T\frac{\Delta u_{i+1}}{\Delta s_{i+1}}\boldsymbol{j}\,.$$

ewton's second law becomes

$$m_i u_i''(t)\boldsymbol{j} = \boldsymbol{T}^+ + \boldsymbol{T}^-,$$

hich gives the component equations

$$T\frac{\Delta x}{\Delta s_i} = T\frac{\Delta x}{\Delta s_{i+1}}, \tag{113}$$

$$m_i u_i''(t) = T\frac{\Delta u_{i+1}}{\Delta s_{i+1}} - T\frac{\Delta u_i}{\Delta s_i}\,. \tag{114}$$

A basic reasonable assumption for a string is small displacements u_i and nall displacement gradients $\Delta u_i/\Delta x$. For small $g = \Delta u_i/\Delta x$ we have that

$$\Delta s_i = \sqrt{\Delta u_i^2 + \Delta x^2} = \Delta x\sqrt{1+g^2} + \Delta x(1 + \frac{1}{2}g^2 + \mathcal{O}(g^4) \approx \Delta x\,.$$

quation (113) is then simply the identity $T = T$, while (114) can be written as

$$m_i u_i''(t) = T\frac{\Delta u_{i+1}}{\Delta x} - T\frac{\Delta u_i}{\Delta x},$$

hich upon division by Δx and introducing the density $\varrho_i = m_i/\Delta x$ becomes

$$\varrho_i u_i''(t) = T\frac{1}{\Delta x^2}\left(u_{i+1} - 2u_i + u_{i-1}\right)\,. \tag{115}$$

/e can now choose to approximate u_i'' by a finite difference in time and get the iscretized wave equation,

$$\varrho_i\frac{1}{\Delta t^2}\left(u_i^{n+1} - 2u_i^n - u_i^{n-1}\right) = T\frac{1}{\Delta x^2}\left(u_{i+1} - 2u_i + u_{i-1}\right)\,. \tag{116}$$

n the other hand, we may go to the continuum limit $\Delta x \to 0$ and replace $u_i(t)$ y $u(x,t)$, ϱ_i by $\varrho(x)$, and recognize that the right-hand side of (115) approaches $^2u/\partial x^2$ as $\Delta x \to 0$. We end up with the continuous model for waves on a ring:

$$\varrho\frac{\partial^2 u}{\partial t^2} = T\frac{\partial^2 u}{\partial x^2}\,.$$

Note that the density ϱ may change along the string, while the tensio constant. With variable wave velocity $c(x) = \sqrt{T/\varrho(x)}$ we can write t equation in the more standard form

$$\frac{\partial^2 u}{\partial t^2} = c^2(x)\frac{\partial^2 u}{\partial x^2}\,.$$

Because of the way ϱ enters the equations, the variable wave velocity c appear inside the derivatives as in many other versions of the wave e However, most strings of interest have constant ϱ.

The end point of a string are fixed so that the displacement u is ze boundary conditions are therefore $u = 0$.

Damping. Air resistance and non-elastic effects in the string will co to reduce the amplitudes of the waves so that the motion dies out aft time. This damping effect can be modeled by a term bu_t on the left-han the equation

$$\varrho\frac{\partial^2 u}{\partial t^2} + b\frac{\partial u}{\partial t} = T\frac{\partial^2 u}{\partial x^2}\,.$$

The parameter b must normally be determined from physical experime

External forcing. It is easy to include an external force acting on th Say we have a vertical force $\tilde{f}_i\boldsymbol{j}$ acting on mass m_i. This force aff vertical component of Newton's law and gives rise to an extra ter on the right-hand side of (117). In the model (118) we would add $f(x,t) = \tilde{f}(x,y)/\varrho(x)$.

Modeling the tension via springs. We assumed, in the derivatio that the tension in the string, T, was constant. It is easy to check this ass by modeling the string segments between the masses as standard spring the force (tension T) is proportional to the elongation of the spring s Let k be the spring constant, and set $T_i = k\Delta\ell$ for the tension in th segment between x_{i-1} and x_i, where $\Delta\ell$ is the elongation of this segme the tension-free state. A basic feature of a string is that it has high te the equilibrium position $u = 0$. Let the string segment have an elongat in the equilibrium position. After deformation of the string, the elong $\Delta\ell = \Delta\ell_0 + \Delta s_i$: $T_i = k(\Delta\ell_0 + \Delta s_i) \approx k(\Delta\ell_0 + \Delta x)$. This shows th independent of i. Moreover, the extra approximate elongation Δx is ve compared to $\Delta\ell_0$, so we may well set $T_i = T = k\Delta\ell_0$. This means t tension is completely dominated by the initial tension determined by th of the string. The additional deformations of the spring during the vi do not introduce significant changes in the tension.

9.2 Waves on a membrane

9.3 Elastic waves in a rod

onsider an elastic rod subject to a hammer impact at the end. This experiment ill give rise to an elastic deformation pulse that travels through the rod. A ıathematical model for longitudinal waves along an elastic rod starts with the eneral equation for deformations and stresses in an elastic medium,

$$\varrho \boldsymbol{u}_{tt} = \nabla \cdot \boldsymbol{\sigma} + \varrho \boldsymbol{f}, \tag{120}$$

here ϱ is the density, $\boldsymbol{u}$ the displacement field, $\boldsymbol{\sigma}$ the stress tensor, and $\boldsymbol{f}$ body orces. The latter has normally no impact on elastic waves.

For stationary deformation of an elastic rod, one has that $\sigma_{xx} = Eu_x$, with ll other stress components being zero. Moreover, $\boldsymbol{u} = u(x)\boldsymbol{i}$. The parameter E known as Young's modulus. Assuming that this simple stress and deformation eld, which is exact in the stationary case, is a good approximation in the ransient case with wave motion, (120) simplifies to

$$\varrho \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(E\frac{\partial u}{\partial x}\right). \tag{121}$$

The associated boundary conditions are u or $\sigma_{xx} = Eu_x$ known, typically $= 0$ for a clamped end and $\sigma_{xx} = 0$ for a free end.

9.4 The acoustic model for seismic waves

eismic waves are used to infer properties of subsurface geological structures. he physical model is a heterogeneous elastic medium where sound is propagated y small elastic vibrations. The general mathematical model for deformations in n elastic medium is based on Newton's second law,

$$\varrho \boldsymbol{u}_{tt} = \nabla \cdot \boldsymbol{\sigma} + \varrho \boldsymbol{f}, \tag{122}$$

nd a constitutive law relating $\boldsymbol{\sigma}$ to $\boldsymbol{u}$, often Hooke's generalized law,

$$\boldsymbol{\sigma} = K\nabla \cdot \boldsymbol{u}\, \boldsymbol{I} + G(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T - \frac{2}{3}\nabla \cdot \boldsymbol{u}\, \boldsymbol{I}). \tag{123}$$

ere, $\boldsymbol{u}$ is the displacement field, $\boldsymbol{\sigma}$ is the stress tensor, $\boldsymbol{I}$ is the identity tensor, ϱ the medium's density, $\boldsymbol{f}$ are body forces (such as gravity), K is the medium's ulk modulus and G is the shear modulus. All these quantities may vary in ɔace, while $\boldsymbol{u}$ and $\boldsymbol{\sigma}$ will also show significant variation in time during wave ıotion.

The acoustic approximation to elastic waves arises from a basic assumption ıat the second term in Hooke's law, representing the deformations that give se to shear stresses, can be neglected. This assumption can be interpreted as pproximating the geological medium by a fluid. Neglecting also the body forces , (122) becomes

$$\varrho \boldsymbol{u}_{tt} = \nabla(K\nabla \cdot \boldsymbol{u})$$

Introducing p as a pressure via

$$p = -K\nabla \cdot \boldsymbol{u},$$

and dividing (124) by ϱ, we get

$$\boldsymbol{u}_{tt} = -\frac{1}{\varrho}\nabla p\,.$$

Taking the divergence of this equation, using $\nabla \cdot \boldsymbol{u} = -p/K$ from (12ɜ the *acoustic approximation to elastic waves*:

$$p_{tt} = K\nabla \cdot \left(\frac{1}{\varrho}\nabla p\right).$$

This is a standard, linear wave equation with variable coefficients. It is ɔ to add a source term $s(x, y, z, t)$ to model the generation of sound wave

$$p_{tt} = K\nabla \cdot \left(\frac{1}{\varrho}\nabla p\right) + s\,.$$

A common additional approximation of (128) is based on using tł rule on the right-hand side,

$$K\nabla \cdot \left(\frac{1}{\varrho}\nabla p\right) = \frac{K}{\varrho}\nabla^2 p + K\nabla\left(\frac{1}{\varrho}\right)\cdot\nabla p \approx \frac{K}{\varrho}\nabla^2 p,$$

under the assumption that the relative spatial gradient $\nabla\varrho^{-1} = -\varrho^{-2}\nabla\varrho$ This approximation results in the simplified equation

$$p_{tt} = \frac{K}{\varrho}\nabla^2 p + s\,.$$

The acoustic approximations to seismic waves are used for sound v the ground, and the Earth's surface is then a boundary where p eqı atmospheric pressure p_0 such that the boundary condition becomes $p =$

Anisotropy. Quite often in geological materials, the effective wave $c = \sqrt{K/\varrho}$ is different in different spatial directions because geological la compacted such that the properties in the horizontal and vertical directiɔ With z as the vertical coordinate, we can introduce a vertical wave vel and a horizontal wave velocity c_h, and generalize (129) to

$$p_{tt} = c_z^2 p_{zz} + c_h^2(p_{xx} + p_{yy}) + s\,.$$

9.5 Sound waves in liquids and gases

ound waves arise from pressure and density variations in fluids. The starting oint of modeling sound waves is the basic equations for a compressible fluid here we omit viscous (frictional) forces, body forces (gravity, for instance), and emperature effects:

$$\varrho_t + \nabla\cdot(\varrho\boldsymbol{u}) = 0, \tag{131}$$
$$\varrho\boldsymbol{u}_t + \varrho\boldsymbol{u}\cdot\nabla\boldsymbol{u} = -\nabla p, \tag{132}$$
$$\varrho = \varrho(p)\,. \tag{133}$$

hese equations are often referred to as the Euler equations for the motion of a uid. The parameters involved are the density ϱ, the velocity $\boldsymbol{u}$, and the pressure . Equation (132) reflects mass balance, (131) is Newton's second law for a fluid, ith frictional and body forces omitted, and (133) is a constitutive law relating ensity to pressure by thermodynamics considerations. A typical model for (133) the so-called isentropic relation[30], valid for adiabatic processes where there is o heat transfer:

$$\varrho = \varrho_0\left(\frac{p}{p_0}\right)^{1/\gamma}. \tag{134}$$

ere, p_0 and ϱ_0 are references values for p and ϱ when the fluid is at rest, and γ the ratio of specific heat at constant pressure and constant volume ($\gamma = 5/3$ r air).

The key approximation in a mathematical model for sound waves is to assume at these waves are small perturbations to the density, pressure, and velocity. /e therefore write

$$p = p_0 + \hat{p},$$
$$\varrho = \varrho_0 + \hat{\varrho},$$
$$\boldsymbol{u} = \hat{\boldsymbol{u}},$$

here we have decomposed the fields in a constant equilibrium value, corre- onding to $\boldsymbol{u} = 0$, and a small perturbation marked with a hat symbol. By serting these decompositions in (131) and (132), neglecting all product terms f small perturbations and/or their derivatives, and dropping the hat symbols, ne gets the following linearized PDE system for the small perturbations in ensity, pressure, and velocity:

$$\varrho_t + \varrho_0\nabla\cdot\boldsymbol{u} = 0, \tag{135}$$
$$\varrho_0\boldsymbol{u}_t = -\nabla p\,. \tag{136}$$

[30] http://en.wikipedia.org/wiki/Isentropic_process

Now we can eliminate ϱ_t by differentiating the relation $\varrho(p)$,

$$\varrho_t = \varrho_0\frac{1}{\gamma}\left(\frac{p}{p_0}\right)^{1/\gamma-1}\frac{1}{p_0}p_t = \frac{\varrho_0}{\gamma p_0}\left(\frac{p}{p_0}\right)^{1/\gamma-1}p_t\,.$$

The product term $p^{1/\gamma-1}p_t$ can be linearized as $p_0^{1/\gamma-1}p_t$, resulting in

$$\varrho_t \approx \frac{\varrho_0}{\gamma p_0}p_t\,.$$

We then get

$$p_t + \gamma p_0\nabla\cdot\boldsymbol{u} = 0,$$
$$\boldsymbol{u}_t = -\frac{1}{\varrho_0}\nabla p,\,.$$

Taking the divergence of (138) and differentiating (137) with respect gives the possibility to easily eliminate $\nabla\cdot\boldsymbol{u}_t$ and arrive at a standarc wave equation for p:

$$p_{tt} = c^2\nabla^2 p,$$

where $c = \sqrt{\gamma p_0/\varrho_0}$ is the speed of sound in the fluid.

19.6 Spherical waves

Spherically symmetric three-dimensional waves propagate in the radial d r only so that $u = u(r,t)$. The fully three-dimensional wave equation

$$\frac{\partial^2 u}{\partial t^2} = \nabla\cdot(c^2\nabla u) + f$$

then reduces to the spherically symmetric wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(c^2(r)r^2\frac{\partial u}{\partial t}\right) + f(r,t), \quad r\in(0,R),\ t>0\,.$$

One can easily show that the function $v(r,t) = ru(r,t)$ fulfills a standa equation in Cartesian coordinates if c is constant. To this end, insert $u =$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(c^2(r)r^2\frac{\partial u}{\partial t}\right)$$

to obtain

$$r\left(\frac{dc^2}{dr}\frac{\partial v}{\partial r} + c^2\frac{\partial^2 v}{\partial r^2}\right) - \frac{dc^2}{dr}v\,.$$

The two terms in the parenthesis can be combined to

$$r\frac{\partial}{\partial r}\left(c^2\frac{\partial v}{\partial r}\right),$$

hich is recognized as the variable-coefficient Laplace operator in one Cartesian oordinate. The spherically symmetric wave equation in terms of $v(r,t)$ now ecomes

$$\frac{\partial^2 v}{\partial t^2} = \frac{\partial}{\partial r}\left(c^2(r)\frac{\partial v}{\partial r}\right) - \frac{1}{r}\frac{dc^2}{dr}v + rf(r,t), \quad r \in (0,R),\ t > 0\,. \tag{141}$$

ı the case of constant wave velocity c, this equation reduces to the wave equation ı a single Cartesian coordinate called r:

$$\frac{\partial^2 v}{\partial t^2} = c^2\frac{\partial^2 v}{\partial r^2} + rf(r,t), \quad r \in (0,R),\ t > 0\,. \tag{142}$$

hat is, any program for solving the one-dimensional wave equation in a Cartesian oordinate system can be used to solve (142), provided the source term is ıultiplied by the coordinate, and that we divide the Cartesian mesh solution by to get the spherically symmetric solution. Moreover, if $r = 0$ is included in the omain, spherical symmetry demands that $\partial u/\partial r = 0$ at $r = 0$, which means ıat

$$\frac{\partial u}{\partial r} = \frac{1}{r^2}\left(r\frac{\partial v}{\partial r} - v\right) = 0, \quad r = 0,$$

nplying $v(0,t) = 0$ as a necessary condition. For practical applications, we xclude $r = 0$ from the domain and assume that some boundary condition is ssigned at $r = \epsilon$, for some $\epsilon > 0$.

9.7 The linear shallow water equations

he next example considers water waves whose wavelengths are much lager than ıe depth and whose wave amplitudes are small. This class of waves may be enerated by catastrophic geophysical events, such as earthquakes at the sea ottom, landslides moving into water, or underwater slides (or a combination, s earthquakes frequently release avalanches of masses). For example, a subsea arthquake will normally have an extension of many kilometers but lift the water nly a few meters. The wave length will have a size dictated by the earthquake rea, which is much lager than the water depth, and compared to this wave ngth, an amplitude of a few meters is very small. The water is essentially a thin lm, and mathematically we can average the problem in the vertical direction nd approximate the 3D wave phenomenon by 2D PDEs. Instead of a moving ater domain in three space dimensions, we get a horizontal 2D domain with an nknown function for the surface elevation and the water depth as a variable oefficient in the PDEs.

Let $\eta(x,y,t)$ be the elevation of the water surface, $H(x,y)$ the water depth orresponding to a flat surface ($\eta = 0$), $u(x,y,t)$ and $v(x,y,t)$ the depth-averaged orizontal velocities of the water. Mass and momentum balance of the water olume give rise to the PDEs involving these quantities:

$$\eta_t = -(Hu)_x - (Hv)_x$$
$$u_t = -g\eta_x,$$
$$v_t = -g\eta_y,$$

where g is the acceleration of gravity. Equation (143) corresponds t balance while the other two are derived from momentum balance (N second law).

The initial conditions associated with (143)-(145) are η, u, and v pr at $t = 0$. A common condition is to have some water elevation $\eta = I(x$ assume that the surface is at rest: $u = v = 0$. A subsea earthquake means a sufficiently rapid motion of the bottom and the water volum that the bottom deformation is mirrored at the water surface as an in $I(x,y)$ and that $u = v = 0$.

Boundary conditions may be η prescribed for incoming, known w zero normal velocity at reflecting boundaries (steep mountains, for in $un_x + vn_y = 0$, where (n_x, n_y) is the outward unit normal to the boundar sophisticated boundary conditions are needed when waves run up at th and at open boundaries where we want the waves to leave the compu domain undisturbed.

Equations (143), (144), and (145) can be transformed to a standar wave equation. First, multiply (144) and (145) by H, differentiate (14 respect to x and (145) with respect to y. Second, differentiate (14 respect to t and use that $(Hu)_{xt} = (Hu_t)_x$ and $(Hv)_{yt} = (Hv_t)_y$ wh independent of t. Third, eliminate $(Hu_t)_x$ and $(Hv_t)_y$ with the aid of th two differentiated equations. These manipulations results in a standar wave equation for η:

$$\eta_{tt} = (gH\eta_x)_x + (gH\eta_y)_y = \nabla\cdot(gH\nabla\eta)\,.$$

In the case we have an initial non-flat water surface at rest, th conditions become $\eta = I(x,y)$ and $\eta_t = 0$. The latter follows from $u = v = 0$, or simply from the fact that the vertical velocity of the surfa which is zero for a surface at rest.

The system (143)-(145) can be extended to handle a time-varying topography, which is relevant for modeling long waves generated by und slides. In such cases the water depth function H is also a function of t the moving slide, and one must add a time-derivative term H_t to the le side of (143). A moving bottom is best described by introducing $z = H$ still-water level, $z = B(x,y,t)$ as the time- and space-varying bottom top so that $H = H_0 - B(x,y,t)$. In the elimination of u and v one may assu the dependence of H on t can be neglected in the terms $(Hu)_{xt}$ and $(Hv$ then end up with a source term in (146), because of the moving (accel bottom:

$$\eta_{tt} = \nabla\cdot(gH\nabla\eta) + B_{tt}\,.$$

The reduction of (147) to 1D, for long waves in a straight channel, or for pproximately plane waves in the ocean, is trivial by assuming no change in y irection ($\partial/\partial y = 0$):

$$\eta_t = (gH\eta_x)_x + B_{tt}\,. \tag{148}$$

Vind drag on the surface. Surface waves are influenced by the drag of the ind, and if the wind velocity some meters above the surface is (U, V), the wind rag gives contributions $C_V\sqrt{U^2+V^2}U$ and $C_V\sqrt{U^2+V^2}V$ to (144) and (145), espectively, on the right-hand sides.

Bottom drag. The waves will experience a drag from the bottom, often oughly modeled by a term similar to the wind drag: $C_B\sqrt{u^2+v^2}u$ on the ght-hand side of (144) and $C_B\sqrt{u^2+v^2}v$ on the right-hand side of (145). Note hat in this case the PDEs (144) and (145) become nonlinear and the elimination f u and v to arrive at a 2nd-order wave equation for η is not possible anymore.

Effect of the Earth's rotation. Long geophysical waves will often be affected y the rotation of the Earth because of the Coriolis force. This force gives rise o a term fv on the right-hand side of (144) and $-fu$ on the right-hand side f (145). Also in this case one cannot eliminate u and v to work with a single quation for η. The Coriolis parameter is $f = 2\Omega\sin\phi$, where Ω is the angular elocity of the earth and ϕ is the latitude.

9.8 Waves in blood vessels

he flow of blood in our bodies is basically fluid flow in a network of pipes. nlike rigid pipes, the walls in the blood vessels are elastic and will increase heir diameter when the pressure rises. The elastic forces will then push the wall ack and accelerate the fluid. This interaction between the flow of blood and the eformation of the vessel wall results in waves traveling along our blood vessels.

A model for one-dimensional waves along blood vessels can be derived from veraging the fluid flow over the cross section of the blood vessels. Let x be a oordinate along the blood vessel and assume that all cross sections are circular, hough with different radius $R(x,t)$. The main quantities to compute is the ross section area $A(x,t)$, the averaged pressure $P(x,t)$, and the total volume ux $Q(x,t)$. The area of this cross section is

$$A(x,t) = 2\pi\int_0^{R(x,t)} r dr, \tag{149}$$

et $v_x(x,t)$ be the velocity of blood averaged over the cross section at point x. he volume flux, being the total volume of blood passing a cross section per me unit, becomes

$$Q(x,t) = A(x,t)v_x(x,t) \tag{150}$$

Mass balance and Newton's second law lead to the PDEs

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = 0,$$
$$\frac{\partial Q}{\partial t} + \frac{\gamma+2}{\gamma+1}\frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right) + \frac{A}{\varrho}\frac{\partial P}{\partial x} = -2\pi(\gamma+2)\frac{\mu}{\varrho}\frac{Q}{A},$$

where γ is a parameter related to the velocity profile, ϱ is the density o and μ is the dynamic viscosity of blood.

We have three unknowns A, Q, and P, and two equations (151) an A third equation is needed to relate the flow to the deformations of the common form for this equation is

$$\frac{\partial P}{\partial t} + \frac{1}{C}\frac{\partial Q}{\partial x} = 0,$$

where C is the compliance of the wall, given by the constitutive relatio

$$C = \frac{\partial A}{\partial P} + \frac{\partial A}{\partial t},$$

which require a relationship between A and P. One common model is the vessel wall, locally, as a thin elastic tube subject to an internal p This gives the relation

$$P = P_0 + \frac{\pi hE}{(1-\nu^2)A_0}(\sqrt{A} - \sqrt{A_0}),$$

where P_0 and A_0 are corresponding reference values when the wall is not d h is the thickness of the wall, and E and ν are Young's modulus and P ratio of the elastic material in the wall. The derivative becomes

$$C = \frac{\partial A}{\partial P} = \frac{2(1-\nu^2)A_0}{\pi hE}\sqrt{A_0} + 2\left(\frac{(1-\nu^2)A_0}{\pi hE}\right)^2 (P - P_0)\,.$$

Another (nonlinear) deformation model of the wall, which has a better experiments, is

$$P = P_0\exp\left(\beta(A/A_0 - 1)\right),$$

where β is some parameter to be estimated. This law leads to

$$C = \frac{\partial A}{\partial P} = \frac{A_0}{\beta P}\,.$$

Reduction to standard wave equation. It is not uncommon to neg viscous term on the right-hand side of (152) and also the quadratic term on the left-hand side. The reduced equations (152) and (153) form a fir linear wave equation system:

$$C\frac{\partial P}{\partial t} = -\frac{\partial Q}{\partial x}, \tag{157}$$

$$\frac{\partial Q}{\partial t} = -\frac{A}{\varrho}\frac{\partial P}{\partial x}\,. \tag{158}$$

hese can be combined into standard 1D wave equation PDE by differentiating ıe first equation with respect t and the second with respect to x,

$$\frac{\partial}{\partial t}\left(CC\frac{\partial P}{\partial t}\right) = \frac{\partial}{\partial x}\left(\frac{A}{\varrho}\frac{\partial P}{\partial x}\right),$$

hich can be approximated by

$$\frac{\partial^2 Q}{\partial t^2} = c^2\frac{\partial^2 Q}{\partial x^2}, \quad c = \sqrt{\frac{A}{\varrho C}}, \tag{159}$$

here the A and C in the expression for c are taken as constant reference values.

9.9 Electromagnetic waves

ight and radio waves are governed by standard wave equations arising from Iaxwell's general equations. When there are no charges and no currents, as in vacuum, Maxwell's equations take the form

$$\nabla\cdot\boldsymbol{E} = 0,$$
$$\nabla\cdot\boldsymbol{B} = 0,$$
$$\nabla\times\boldsymbol{E} = -\frac{\partial\boldsymbol{B}}{\partial t},$$
$$\nabla\times\boldsymbol{B} = \mu_0\epsilon_0\frac{\partial\boldsymbol{E}}{\partial t},$$

here $\epsilon_0 = 8.854187817620\cdot 10^{-12}$ (F/m) is the permittivity of free space, also nown as the electric constant, and $\mu_0 = 1.2566370614\cdot 10^{-6}$ (H/m) is the ermeability of free space, also known as the magnetic constant. Taking the curl f the two last equations and using the identity

$$\nabla\times(\nabla\times\boldsymbol{E}) = \nabla(\nabla\cdot\boldsymbol{E}) - \nabla^2\boldsymbol{E} = -\nabla^2\boldsymbol{E} \text{ when } \nabla\cdot\boldsymbol{E} = 0,$$

nmediately gives the wave equation governing the electric and magnetic field:

$$\frac{\partial^2\boldsymbol{E}}{\partial t^2} = c^2\frac{\partial^2\boldsymbol{E}}{\partial x^2}, \tag{160}$$

$$\frac{\partial^2\boldsymbol{E}}{\partial t^2} = c^2\frac{\partial^2\boldsymbol{E}}{\partial x^2}, \tag{161}$$

ith $c = 1/\sqrt{\mu_0\epsilon_0}$ as the velocity of light. Each component of $\boldsymbol{E}$ and $\boldsymbol{B}$ fulfills a ave equation and can hence be solved independently.

20 Exercises

Exercise 15: Simulate waves on a non-homogeneous s

Simulate waves on a string that consists of two materials with different The tension in the string is constant, but the density has a jump at the m the string. Experiment with different sizes of the jump and produce ani that visualize the effect of the jump on the wave motion.

Hint. According to Section 19.1, the density enters the mathematical m ϱ in $\varrho u_{tt} = Tu_{xx}$, where T is the string tension. Modify, e.g., the `wave1D_` code to incorporate the tension and two density values. Make a mesh f `rho` with density values at each spatial mesh point. A value for the tens be 150 N. Corresponding density values can be computed from the wave estimations in the `guitar` function in the `wave1D_u0v.py` file.
Filename: `wave1D_u0_sv_discont.py`.

Exercise 16: Simulate damped waves on a string

Formulate a mathematical model for damped waves on a string. Use da Section 3.4, and tune the damping parameter so that the string is ve to the rest state after 15 s. Make a movie of the wave motion. Fi `wave1D_u0_sv_damping.py`.

Exercise 17: Simulate elastic waves in a rod

A hammer hits the end of an elastic rod. The exercise is to simulate the m wave motion using the model (121) from Section 19.3. Let the rod hav L and let the boundary $x = L$ be stress free so that $\sigma_{xx} = 0$, implyi $\partial u/\partial x = 0$. The left end $x = 0$ is subject to a strong stress pulse (the h modeled as

$$\sigma_{xx}(t) = \begin{cases} S, & 0 < t \leq t_s, \\ 0, & t > t_s \end{cases}$$

The corresponding condition on u becomes $u_x = S/E$ for $t \leq t_s$ a afterwards (recall that $\sigma_{xx} = Eu_x$). This is a non-homogeneous N condition, and you will need to approximate this condition and combine the scheme (the ideas and manipulations follow closely the handling of a n initial condition $u_t = V$ in wave PDEs or the corresponding second-orde for vibrations). Filename: `wave_rod.py`.

Exercise 18: Simulate spherical waves

Implement a model for spherically symmetric waves using the method d in Section 19.6. The boundary condition at $r = 0$ must be $\partial u/\partial r = 0$, w condition at $r = R$ can either be $u = 0$ or a radiation condition as desc

roblem 21. The $u = 0$ condition is sufficient if R is so large that the amplitude f the spherical wave has become insignificant. Make movie(s) of the case where ıe source term is located around $r = 0$ and sends out pulses

$$f(r,t) = \begin{cases} Q\exp\left(-\frac{r^2}{2\Delta r^2}\right)\sin\omega t, & \sin\omega t \geq 0 \\ 0, & \sin\omega t < 0 \end{cases}$$

ere, Q and ω are constants to be chosen.

lint. Use the program `wave1D_u0v.py` as a starting point. Let `solver` compute the v function and then set $u = v/r$. However, $u = v/r$ for $r = 0$ requires pecial treatment. One possibility is to compute `u[1:] = v[1:]/r[1:]` and ıen set `u[0]=u[1]`. The latter makes it evident that $\partial u/\partial r = 0$ in a plot. ilename: `wave1D_spherical.py`.

xercise 19: Explain why numerical noise occurs

he experiments performed in Exercise 8 shows considerable numerical noise ı the form of non-physical waves, especially for $s_f = 4$ and the plug pulse r the half a "cosinehat" pulse. The noise is much less visible for a Gaussian ulse. Run the case with the plug and half a "cosinehat" pulses for $s_f = 1$, $' = 0.9, 0.25$, and $N_x = 40, 80, 160$. Use the numerical dispersion relation to xplain the observations. Filename: `pulse1D_analysis.pdf`.

xercise 20: Investigate harmonic averaging in a 1D model

armonic means are often used if the wave velocity is non-smooth or discon- nuous. Will harmonic averaging of the wave velocity give less numerical oise for the case $s_f = 4$ in Exercise 8? Filenames: `pulse1D_harmonic.pdf`, `ulse1D_harmonic.py`.

roblem 21: Implement open boundary conditions

o enable a wave to leave the computational domain and travel undisturbed ırough the boundary $x = L$, one can in a one-dimensional problem impose the ollowing condition, called a *radiation condition* or *open boundary condition*:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0\,. \tag{162}$$

he parameter c is the wave velocity.

Show that (162) accepts a solution $u = g_R(x - ct)$ (right-going wave), but ot $u = g_L(x + ct)$ (left-going wave). This means that (162) will allow any ght-going wave $g_R(x - ct)$ to pass through the boundary undisturbed.

A corresponding open boundary condition for a left-going wave through $x = 0$

$$\frac{\partial u}{\partial t} - c\frac{\partial u}{\partial x} = 0\,.$$

a) A natural idea for discretizing the condition (162) at the spatial er $i = N_x$ is to apply centered differences in time and space:

$$[D_{2t}u + cD_{2x}u = 0]_i^n, \quad i = N_x\,.$$

Eliminate the fictitious value $u^n_{N_x+1}$ by using the discrete equation at t point.

The equation for the first step, u_i^1, is in principle also affected, but then use the condition $u_{N_x} = 0$ since the wave has not yet reached t boundary.

b) A much more convenient implementation of the open boundary conc $x = L$ can be based on an explicit discretization

$$[D_t^+u + cD_x^-u = 0]_i^n, \quad i = N_x\,.$$

From this equation, one can solve for $u^{n+1}_{N_x}$ and apply the formula as a I condition at the boundary point. However, the finite difference approxi involved are of first order.

Implement this scheme for a wave equation $u_{tt} = c^2u_{xx}$ in a domai where you have $u_x = 0$ at $x = 0$, the condition (162) at $x = L$, and a disturbance in the middle of the domain, e.g., a plug profile like

$$u(x,0) = \begin{cases} 1, & L/2 - \ell \leq x \leq L/2 + \ell, \\ 0, \text{otherwise} \end{cases}$$

Observe that the initial wave is split in two, the left-going wave is refl $x = 0$, and both waves travel out of $x = L$, leaving the solution as $u = 0$ Use a unit Courant number such that the numerical solution is exact. movie to illustrate what happens.

Because this simplified implementation of the open boundary conditio there is no need to pursue the more complicated discretization in a).

Hint. Modify the solver function in `wave1D_dn.py`[31].

c) Add the possibility to have either $u_x = 0$ or an open boundary conc the left boundary. The latter condition is discretized as

$$[D_t^+u - cD_x^+u = 0]_i^n, \quad i = 0,$$

leading to an explicit update of the boundary value u_0^{n+1}.

The implementation can be tested with a Gaussian function as initi tion:

[31] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_dn.py`

$$g(x; m, s) = \frac{1}{\sqrt{2\pi}s} e^{-\frac{(x-m)^2}{2s^2}} .$$

un two tests:

1. Disturbance in the middle of the domain, $I(x) = g(x; L/2, s)$, and open boundary condition at the left end.

2. Disturbance at the left end, $I(x) = g(x; 0, s)$, and $u_x = 0$ as symmetry boundary condition at this end.

lake nose tests for both cases, testing that the solution is zero after the waves ave left the domain.

) In 2D and 3D it is difficult to compute the correct wave velocity normal to ıe boundary, which is needed in generalizations of the open boundary conditions ı higher dimensions. Test the effect of having a slightly wrong wave velocity in .65). Make a movies to illustrate what happens.
ilename: `wave1D_open_BC.py`.

emarks. The condition (162) works perfectly in 1D when c is known. In 2D nd 3D, however, the condition reads $u_t + c_x u_x + c_y u_y = 0$, where c_x and c_y re the wave speeds in the x and y directions. Estimating these components .e., the direction of the wave) is often challenging. Other methods are normally sed in 2D and 3D to let waves move out of a computational domain.

xercise 22: Implement periodic boundary conditions

is frequently of interest to follow wave motion over large distances and long mes. A straightforward approach is to work with a very large domain, but ıight lead to a lot of computations in areas of the domain where the waves annot be noticed. A more efficient approach is to let a right-going wave out f the domain and at the same time let it enter the domain on the left. This is alled a *periodic boundary condition*.

The boundary condition at the right end $x = L$ is an open boundary condition ee Exercise 21) to let a right-going wave out of the domain. At the left end, $= 0$, we apply, in the beginning of the simulation, either a symmetry boundary ɔndition (see Exercise 7) $u_x = 0$, or an open boundary condition.

This initial wave will split in two and either reflected or transported out of ıe domain at $x = 0$. The purpose of the exercise is to follow the right-going ave. We can do that with a *periodic boundary condition*. This means that when ıe right-going wave hits the boundary $x = L$, the open boundary condition lets ıe wave out of the domain, but at the same time we use a boundary condition ı the left end $x = 0$ that feeds the outgoing wave into the domain again. This eriodic condition is simply $u(0) = u(L)$. The switch from $u_x = 0$ or an open oundary condition at the left end to a periodic condition can happen when

$u(L, t) > \epsilon$, where $\epsilon = 10^{-4}$ might be an appropriate value for determini the right-going wave hits the boundary $x = L$.

The open boundary conditions can conveniently be discretized as ex in Exercise 21. Implement the described type of boundary conditic test them on two different initial shapes: a plug $u(x, 0) = 1$ for x $u(x, 0) = 0$ for $x > 0.1$, and a Gaussian function in the middle of the $u(x, 0) = \exp(-\frac{1}{2}(x - 0.5)^2/0.05)$. The domain is the unit interval $[0,$ these two shapes for Courant numbers 1 and 0.5. Assume constant wave Make movies of the four cases. Reason why the solutions are correct. F `periodic.py`.

Problem 23: Earthquake-generated tsunami over a s hill

A subsea earthquake leads to an immediate lift of the water surface, see F The lifted water surface splits into two tsunamis, one traveling to the ri one to the left, as depicted in Figure 11. Since tsunamis are normally v waves, compared to the depth, with a small amplitude, compared to t length, the wave equation model described in Section 19.7 is relevant:

$$\eta_{tt} = (gH(x)\eta_x)_x,$$

where g is the acceleration of gravity, and $H(x)$ is the still water depth

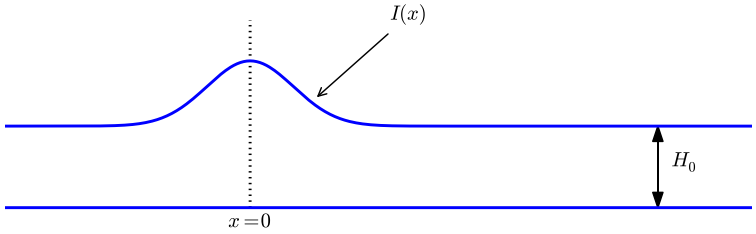


Figure 10: Sketch of initial water surface due to a subsea earthqua

To simulate the right-going tsunami, we can impose a symmetry bc at $x = 0$: $\partial\eta\ \partial x = 0$. We then simulate the wave motion in $[0, L]$. Un ocean ends at $x = L$, the waves should travel undisturbed through the b $x = L$. A radiation condition as explained in Problem 21 can be used purpose. Alternatively, one can just stop the simulations before the w

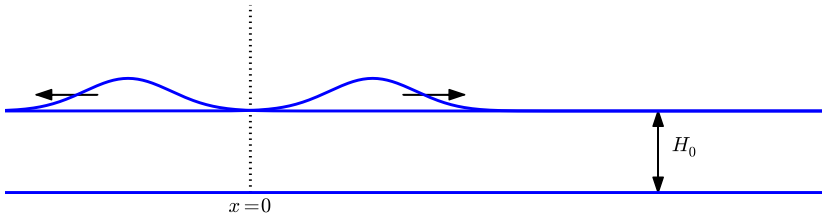


Figure 11: An initial surface elevation is split into two waves.

ıe boundary at $x = L$. In that case it does not matter what kind of boundary ɔndition we use at $x = L$. Imposing $\eta = 0$ and stopping the simulations when $|_i^n| > \epsilon$, $i = N_x - 1$, is a possibility (ϵ is a small parameter).

The shape of the initial surface can be taken as a Gaussian function,

$$I(x; I_0, I_a, I_m, I_s) = I_0 + I_a \exp\left(-\left(\frac{x - I_m}{I_s}\right)^2\right), \tag{167}$$

ith $I_m = 0$ reflecting the location of the peak of $I(x)$ and I_s being a measure f the width of the function $I(x)$ (I_s is $\sqrt{2}$ times the standard deviation of the ıniliar normal distribution curve).

Now we extend the problem with a hill at the sea bottom, see Figure 12. The ave speed $c = \sqrt{gH(x)} = \sqrt{g(H_0 - B(x))}$ will then be reduced in the shallow ater above the hill.

One possible form of the hill is a Gaussian function,

$$B(x; B_0, B_a, B_m, B_s) = B_0 + B_a \exp\left(-\left(\frac{x - B_m}{B_s}\right)^2\right), \tag{168}$$

ut many other shapes are also possible, e.g., a "cosine hat" where

$$B(x; B_0, B_a, B_m, B_s) = B_0 + B_a \cos\left(\pi\frac{x - B_m}{2B_s}\right), \tag{169}$$

hen $x \in [B_m - B_s, B_m + B_s]$ while $B = B_0$ outside this interval.

Also an abrupt construction may be tried:

$$B(x; B_0, B_a, B_m, B_s) = B_0 + B_a, \tag{170}$$

ɔr $x \in [B_m - B_s, B_m + B_s]$ while $B = B_0$ outside this interval.

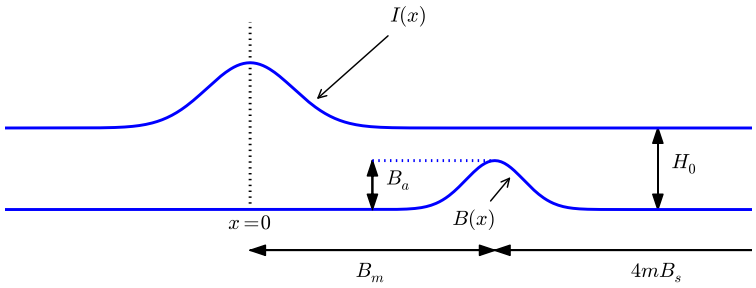


Figure 12: Sketch of an earthquake-generated tsunami passing over a hill.

The `wave1D_dn_vc.py`[32] program can be used as starting point implementation. Visualize both the bottom topography and the water elevation in the same plot. Allow for a flexible choice of bottom shape (169), (170), or $B(x) = B_0$ (flat).

The purpose of this problem is to explore the quality of the numerical η_i^n for different shapes of the bottom obstruction. The "cosine hat" and shaped hills have abrupt changes in the derivative of $H(x)$ and are more generate numerical noise than the smooth Gaussian shape of the hill. Inv if this is true. Filenames: `tsunami1D_hill.py`, `tsunami1D_hill.pdf`.

Problem 24: Earthquake-generated tsunami over a 3

This problem extends Problem 23 to a three-dimensional wave phenc governed by the 2D PDE (146). We assume that the earthquake arise fault along the line $x = 0$ in the xy-plane so that the initial lift of the can be taken as $I(x)$ in Problem 23. That is, a plane wave is propagatin right, but will experience bending because of the bottom.

The bottom shape is now a function of x and y. An "elliptic" G function in two dimensions, with its peak at (B_{mx}, B_{my}), generalizes (1

$$B(x; B_0, B_a, B_{mx}, B_{my}, B_s, b) = B_0 + B_a \exp\left(-\left(\frac{x - B_{mx}}{B_s}\right)^2 - \left(\frac{y - I}{bB}\right.\right.$$

[32] `http://tinyurl.com/nm5587k/wave/wave1D/wave1D_dn_vc.py`

here b is a scaling parameter: $b = 1$ gives a circular Gaussian function with rcular contour lines, while $b \neq 1$ gives an elliptic shape with elliptic contour nes.

The "cosine hat" (169) can also be generalized to

$$B(x; B_0, B_a, B_{mx}, B_{my}, B_s) = B_0 + B_a \cos\left(\pi \frac{x - B_{mx}}{2B_s}\right) \cos\left(\pi \frac{y - B_{my}}{2B_s}\right), \tag{172}$$

hen $0 \leq \sqrt{x^2 + y^2} \leq B_s$ and $B = B_0$ outside this circle.

A box-shaped obstacle means that

$$B(x; B_0, B_a, B_m, B_s, b) = B_0 + B_a \tag{173}$$

or x and y inside a rectangle

$$B_{mx} - B_s \leq x \leq B_{mx} + B_s, \quad B_{my} - bB_s \leq y \leq B_{my} + bB_s,$$

nd $B = B_0$ outside this rectangle. The b parameter controls the rectangular ıape of the cross section of the box.

Note that the initial condition and the listed bottom shapes are symmetric round the line $y = B_{my}$. We therefore expect the surface elevation also to e symmetric with respect to this line. This means that we can halve the omputational domain by working with $[0, L_x] \times [0, B_{my}]$. Along the upper oundary, $y = B_{my}$, we must impose the symmetry condition $\partial\eta/\partial n = 0$. Such symmetry condition ($-\eta_x = 0$) is also needed at the $x = 0$ boundary because ıe initial condition has a symmetry here. At the lower boundary $y = 0$ we also et a Neumann condition (which becomes $-\eta_y = 0$). The wave motion is to be mulated until the wave hits the reflecting boundaries where $\partial\eta/\partial n = \eta_x = 0$ ne can also set $\eta = 0$ - the particular condition does not matter as long as the mulation is stopped before the wave is influenced by the boundary condition).

Visualize the surface elevation. Investigate how different hill shapes, different sizes of the water gap above the hill, and different resolutions $\Delta x = y = h$ and Δt influence the numerical quality of the solution. Filenames: `sunami2D_hill.py`, `tsunami2D_hill.pdf`.

roblem 25: Investigate Matplotlib for visualization

lay with native Matplotlib code for visualizing 2D solutions of the wave equation ith variable wave velocity. See if there are effective ways to visualize both the olution and the wave velocity. Filename: `tsunami2D_hill_mpl.py`.

roblem 26: Investigate visualization packages

reate some fancy 3D visualization of the water waves *and* the subsea hill in roblem 24. Try to make the hill transparent. Possible visualization tools are

- Mayavi[33]
- Paraview[34]
- OpenDX[35]

Filename: `tsunami2D_hill_viz.py`.

Problem 27: Implement loops in compiled languages

Extend the program from Problem 24 such that the loops over mesh point the time loop, are implemented in compiled languages. Consider impleme in Cython, Fortran via `f2py`, C via Cython, C via `f2py`, C/C++ via and C/C++ via `scipy.weave`. Perform efficiency experiments to investi relative performance of the various implementations. It is often advan to normalize CPU times by the fastest method on a given mesh. Fi `tsunami2D_hill_compiled.py`.

Exercise 28: Simulate seismic waves in 2D

The goal of this exercise is to simulate seismic waves using the PDE (130) in a 2D xz domain with geological layers. Introduce m horizonta of thickness h_i, $i = 0, \ldots, m-1$. Inside layer number i we have a vertic velocity $c_{z,i}$ and a horizontal wave velocity $c_{h,i}$. Make a program for sin such 2D waves. Test it on a case with 3 layers where

$$c_{z,0} = c_{z,1} = c_{z,2}, \quad c_{h,0} = c_{h,2}, \quad c_{h,1} \ll c_{h,0}\,.$$

Let s be a localized point source at the middle of the Earth's surfa upper boundary) and investigate how the resulting wave travels thro medium. The source can be a localized Gaussian peak that oscillates for some time interval. Place the boundaries far enough from the exp wave so that the boundary conditions do not disturb the wave. Then t of boundary condition does not matter, except that we physically need $p = p_0$, where p_0 is the atmospheric pressure, at the upper boundary. F `seismic2D.py`.

Project 29: Model 3D acoustic waves in a room

The equation for sound waves in air is derived in Section 19.5 and read

$$p_{tt} = c^2 \nabla^2 p,$$

where $p(x, y, z, t)$ is the pressure and c is the speed of sound, taken as However, sound is absorbed in the air due to relaxation of molecules in

[33] `http://code.enthought.com/projects/mayavi/`
[34] `http://www.paraview.org/`
[35] `http://www.opendx.org/`

. model for simple relaxation, valid for gases consisting only of one type of olecules, is a term $c^2\tau_s\nabla^2 p_t$ in the PDE, where τ_s is the relaxation time. If we enerate sound from, e.g., a loudspeaker in the room, this sound source must lso be added to the governing equation.

The PDE with the mentioned type of damping and source then becomes

$$p_t t = c^2\nabla^p + c^2\tau_s\nabla^2 p_t + f, \tag{174}$$

here $f(x, y, z, t)$ is the source term.

The walls can absorb some sound. A possible model is to have a "wall layer" hicker than the physical wall) outside the room where c is changed such that ome of the wave energy is reflected and some is absorbed in the wall. The bsorption of energy can be taken care of by adding a damping term bp_t in the quation:

$$p_t t + bp_t = c^2\nabla^p + c^2\tau_s\nabla^2 p_t + f\,. \tag{175}$$

ypically, $b = 0$ in the room and $b > 0$ in the wall. A discontinuity in b or c ill give rise to reflections. It can be wise to use a constant c in the wall to ontrol reflections because of the discontinuity between c in the air and in the all, while b is gradually increased as we go into the wall to avoid reflections ecause of rapid changes in b. At the outer boundary of the wall the condition $= 0$ or $\partial p/\partial n = 0$ can be imposed. The waves should anyway be approximately ampened to $p = 0$ this far out in the wall layer.

There are two strategies for discretizing the $\nabla^2 p_t$ term: using a center ifference between times $n + 1$ and $n - 1$ (if the equation is sampled at level n), r use a one-sided difference based on levels n and $n - 1$. The latter has the dvantage of not leading to any equation system, while the former is second-order ccurate as the scheme for the simple wave equation $p_t t = c^2\nabla^2 p$. To avoid an quation system, go for the one-sided difference such that the overall scheme ecomes explicit and only of first order in time.

Develop a 3D solver for the specified PDE and introduce a wall layer. Test the olver with the method of manufactured solutions. Make some demonstrations here the wall reflects and absorbs the waves (reflection because of discontinuity n b and absorption because of growing b). Experiment with the impact of the s parameter. Filename: `acoustics.py`.

roject 30: Solve a 1D transport equation

/e shall study the wave equation

$$u_t + cu_x = 0, \quad x \in (0, L],\ t \in (0, T], \tag{176}$$

ith initial condition

$$u(x, 0) = I(x), \quad x \in [0, L], \tag{177}$$

nd *one* periodic boundary condition

$$u(0, t) = u(L, t)\,.$$

This boundary condition means that what goes out of the domain at comes in at $x = 0$. Roughly speaking, we need only one boundary co because of the spatial derivative is of first order only.

Physical interpretation. The parameter c can be constant or varia $c(x)$. The equation (176) arises in *transport* problems where a quantity u could be temperature or concentration of some contaminant, is transport the velocity c of a fluid. In addition to the transport imposed by "travelli the fluid", u may also be transported by diffusion (such as heat condu Fickian diffusion), but we have in the model $u_t + cu_x$ assumed that d effects are negligible, which they often are.

A widely used numerical scheme for (176) applies a forward differ time and a backward difference in space when $c > 0$:

$$[D_t^+ u + cD_x^- u = 0]_i^n\,.$$

For $c < 0$ we use a forward difference in space: $[cD_x^+ u]_i^n$.

We shall hereafter assume that $= c(x) > 0$.

To compute (184) we need to integrate $1/c$ to obtain C and then c the inverse of C.

The inverse function computation can be easily done if we first think di Say we have some function $y = g(x)$ and seeks its inverse. Plotting where $y_i = g(x_i)$ for some mesh points x_i, displays g as a function of inverse function is simply x as a function of g, i.e., the curve with points We can therefore quickly compute points at the curve of the inverse f One way of extending these points to a continuous function is to assume variation (known as linear interpolation) between the points (which a means to draw straight lines between the points, exactly as done by a program).

The function `wrap2callable` in `scitools.std` can take a set of poi return a continuous function that corresponds to linear variation betw points. The computation of the inverse of a function g on $[0, L]$ can done by

```
def inverse(g, domain, resolution=101):
    x = linspace(domain[0], domain[L], resolution)
    y = g(x)
    from scitools.std import wrap2callable
    g_inverse = wrap2callable((y, x))
    return g_inverse
```

To compute $C(x)$ we need to integrate $1/c$, which can be done by a Tra rule. Suppose we have computed $C(x_i)$ and need to compute $C(x_{i+1})$ the Trapezoidal rule with m subintervals over the integration domain [gives

$$C(x_{i+1}) = C(x_i) + \int_{x_i}^{x_{i+1}} \frac{dx}{c} \approx h\left(\frac{1}{2}\frac{1}{c(x_i)} + \frac{1}{2}\frac{1}{c(x_{i+1})} + \sum_{j=1}^{m-1}\frac{1}{c(x_i+jh)}\right), \tag{180}$$

here $h = (x_{i+1} - x_i)/m$ is the length of the subintervals used for the integral ver $[x_i, x_{i+1}]$. We observe that (180) is a *difference equation* which we can solve y repeatedly applying (180) for $i = 0, 1, \ldots, N_x - 1$ if a mesh $x_0, x_, \ldots, x_{N_x}$ is rescribed. Note that $C(0) = 0$.

) Show that under the assumption of $a = \text{const}$,

$$u(x,t) = I(x - ct) \tag{181}$$

ulfills the PDE as well as the initial and boundary condition (provided $I(0) = (L)$).

) Set up a computational algorithm and implement it in a function. Assume a constant and positive.

) Test implementation by using the remarkable property that the numerical olution is exact at the mesh points if $\Delta t = c^{-1}\Delta x$.

) Make a movie comparing the numerical and exact solution for the following wo choices of initial conditions:

$$I(x) = \left[\sin\left(\pi\frac{x}{L}\right)\right]^{2n} \tag{182}$$

here n is an integer, typically $n = 5$, and

$$I(x) = \exp\left(-\frac{(x - L/2)^2}{2\sigma 2}\right). \tag{183}$$

Choose $\Delta t = c^{-1}\Delta x, 0.9c^{-1}\Delta x, 0.5c^{-1}\Delta x$.

) The performance of the suggested numerical scheme can be investigated y analyzing the numerical dispersion relation. Analytically, we have that the *ourier component*

$$u(x,t) = e^{i(kx - \omega t)},$$

a solution of the PDE if $\omega = kc$. This is the *analytical dispersion relation*. A omplete solution of the PDE can be built by adding up such Fourier components ith different amplitudes, where the initial condition I determines the amplitudes. he solution u is then represented by a Fourier series.

A similar discrete Fourier component at (x_p, t_n) is

$$u_p^q = e^{i(kp\Delta x - \tilde{\omega} n\Delta t)},$$

where in general $\tilde{\omega}$ is a function of k, Δt, and Δx, and differs from tl $\omega = kc$.

Insert the discrete Fourier component in the numerical scheme and d expression for $\tilde{\omega}$, i.e., the discrete dispersion relation. Show in particu if the $\Delta t/(c\Delta x) = 1$, the discrete solution coincides with the exact sol the mesh points, regardless of the mesh resolution (!). Show that if the condition

$$\frac{\Delta t}{c\Delta x} \leq 1,$$

the discrete Fourier component cannot grow (i.e., $\tilde{\omega}$ is real).

f) Write a test for your implementation where you try to use informati the numerical dispersion relation.

g) Set up a computational algorithm for the variable coefficient case plement it in a function. Make a test that the function works for c a.

h) It can be shown that for an observer moving with velocity $c(x)$, u is c This can be used to derive an exact solution when a varies with x. Sh that

$$u(x,t) = f(C(x) - t),$$

where

$$C'(x) = \frac{1}{c(x)},$$

is a solution of (176) for any differentiable function f.

i) Use the initial condition to show that an exact solution is

$$u(x,t) = I(C^{-1}(C(x) - t)),$$

with C^{-1} being the inverse function of $C = \int c^1 dx$. Since $C(x)$ is an $\int_0^x (1/c)dx$, $C(x)$ is monotonically increasing and there exists hence an function C^{-1} with values in $[0, L]$.

j) Implement a function for computing $C(x_i)$ and one for computing C^- any x. Use these two functions for computing the exact solution $I(C^{-1}(C$ End up with a function `u_exact_variable_c(x, n, c, I)` that retu value of $I(C^{-1}(C(x) - t_n))$.

) Make movies showing a comparison of the numerical and exact solutions for
ıe two initial conditions (182) and (30). Choose $\Delta t = \Delta x/\max_{0,L} c(x)$ and the
elocity of the medium as

1. $c(x) = 1 + \epsilon \sin(k\pi x/L)$, $\epsilon < 1$,
2. $c(x) = 1 + I(x)$, where I is given by (182) or (30).

he PDE $u_t + cu_x = 0$ expresses that the initial condition $I(x)$ is transported
ith velocity $c(x)$.
ilename: `advec1D.py`.

roblem 31: General analytical solution of a 1D damped ave equation

/e consider an initial-boundary value problem for the damped wave equation:

$$
\begin{aligned}
u_{tt} + bu_t &= c^2 u_{xx}, && x \in (0,L),\ t \in (0,T] \\
u(0,t) &= 0, \\
u(L,t) &= 0, \\
u(x,0) &= I(x), \\
u_t(x,0) &= V(x)\,.
\end{aligned}
$$

ere, $b \geq 0$ and c are given constants. The aim is to derive a general analytical
olution of this problem. Familiarity with the method of separation of variables
or solving PDEs will be assumed.

) Seek a solution on the form $u(x,t) = X(x)T(t)$. Insert this solution in the
DE and show that it leads to two differential equations for X and T:

$$T'' + bT' + \lambda T = 0, \quad c^2 X'' + \lambda X = 0,$$

ith $X(0) = X(L) = 0$ as boundary conditions, and λ as a constant to be
etermined.

) Show that $X(x)$ is on the form

$$X_n(x) = C_n \sin kx, \quad k = \frac{n\pi}{L}, \quad n = 1, 2, \ldots$$

here C_n is an arbitrary constant.

) Under the assumption that $(b/2)^2 < k^2$, show that $T(t)$ is on the form

$$T_n(t) = e^{-\frac{1}{2}bt}(a_n \cos\omega t + b_n \sin\omega t), \quad \omega = \sqrt{k^2 - \frac{1}{4}b^2}, \quad n = 1, 2, \ldots$$

he complete solution is then

$$u(x,t) = \sum_{n=1}^{\infty} \sin kx e^{-\frac{1}{2}bt}(A_n \cos\omega t + B_n \sin\omega t),$$

where the constants A_n and B_n must be computed from the initial con

d) Derive a formula for A_n from $u(x,0) = I(x)$ and developing $I(x)$ a
Fourier series on $[0, L]$.

e) Derive a formula for B_n from $u_t(x,0) = V(x)$ and developing $V(x)$ ε
Fourier series on $[0, L]$.

f) Calculate A_n and B_n from vibrations of a string where $V(x) = 0$ an

$$I(x) = \begin{cases} ax/x_0, & x < x_0, \\ a(L-x)/(L-x_0), & \text{otherwise} \end{cases}$$

g) Implement the series for $u(x,t)$ in a function `u_series(x, t, tol=`
where `tol` is a tolerance for truncating the series. Simply sum the terı
$|a_n|$ and $|b_b|$ both are less than `tol`.

h) What will change in the derivation of the analytical solution if ı
$u_x(0,t) = u_x(L,t) = 0$ as boundary conditions? And how will you sc
problem with $u(0,t) = 0$ and $u_x(L,t) = 0$?
Filename: `damped_wave1D.pdf`.

Problem 32: General analytical solution of a 2D da wave equation

Carry out Problem 31 in the 2D case: $u_{tt} + bu_t = c^2(u_{xx} + u_{yy})$, where
$(0, L_x) \times (0, L_y)$. Assume a solution on the form $u(x,y,t) = X(x)Y$
Filename: `damped_wave2D.pdf`.

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